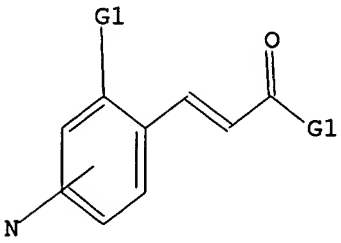
Uploading C:\Program Files\Stnexp\Queries\323.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



G1 O,S,NH

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

FULL SEARCH INITIATED 13:28:10 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 28505 TO ITERATE

100.0% PROCESSED 28505 ITERATIONS 1836 ANSWERS
SEARCH TIME: 00.00.01

L2 1836 SEA SSS FUL L1

L3 278 L2

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L4 216 L2 AND PY<2001

=> s l4 and heterocy?
150269 HETEROCY?
L5 22 L4 AND HETEROCY?

=> d 1-22 ibib abs hitstr

L5 ANSWER 1 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2000:573791 CAPLUS
DOCUMENT NUMBER: 133:164009
TITLE: Preparation of phenyl ureas and thioureas as orexin receptor antagonists
INVENTOR(S): Coulton, Steven; Johns, Amanda; Porter, Roderick Alan
PATENT ASSIGNEE(S): Smithkline Beecham Plc, UK

SOURCE: PCT Int. Appl., 45 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000047577	A1	20000817	WO 2000-EP1150		20000210 <--
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
EP 1150977	A1	20011107	EP 2000-906324		20000210
EP 1150977	B1	20040825			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2002536445	T2	20021029	JP 2000-598497		20000210
AT 274512	E	20040915	AT 2000-906324		20000210
ES 2226785	T3	20050401	ES 2000-906324		20000210
US 6699879	B1	20040302	US 2002-913236		20020429
PRIORITY APPLN. INFO.:			GB 1999-3266	A	19990212
			GB 1999-26430	A	19991108
			WO 2000-EP1150	W	20000210

OTHER SOURCE(S): MARPAT 133:164009
GI

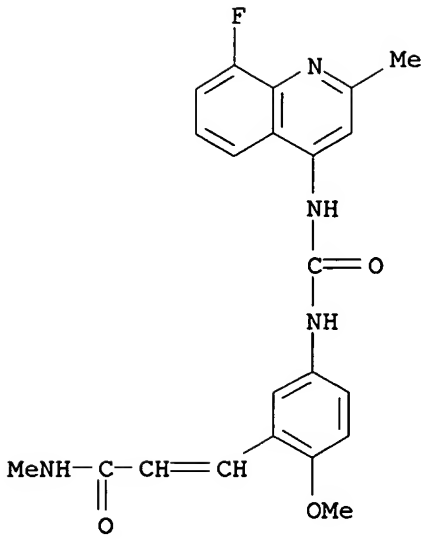
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; Z = O, S; R1 = alkyl, alkenyl, alkoxy, etc.; R2-R6 = alkyl, alkenyl, alkoxy, etc.; adjacent pair of R2-R6 together with the carbon atoms to which they are attached form (un)substituted carbocyclyl, **heterocyclyl**; R7 = alkyl, alkenyl, alkoxy, etc.; n = 0-3] and their pharmaceutically acceptable salts which are non-peptide antagonists of human orexin receptors, in particular orexin-1 receptors, were prepared E.g., treatment of 4-amino-2-methylquinoline with carbonyl diimidazole in CH2Cl2 followed by addition of 6-amino-2-methylbenzoxazole afforded II which showed pKb > 6.0 against orexin-1 receptor. In particular, compds. I are of potential use in the treatment of obesity including obesity observed in Type 2(non-insulin-dependent) diabetes patients and/or sleep disorders.

IT **288150-79-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of Ph ureas and thioureas as orexin receptor antagonists)

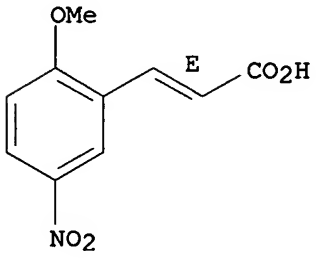
RN 288150-79-8 CAPLUS

CN 2-Propenamide, 3-[5-[[[(8-fluoro-2-methyl-4-quinolinyl)amino]carbonyl]amino]-2-methoxyphenyl]-N-methyl- (9CI) (CA INDEX NAME)



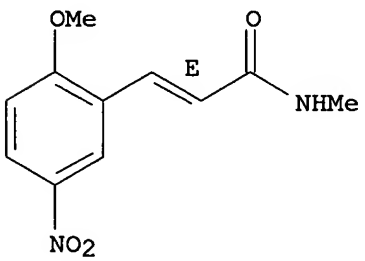
IT **288151-91-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of Ph ureas and thioureas as orexin receptor antagonists)
RN 288151-91-7 CAPLUS
CN 2-Propenoic acid, 3-(2-methoxy-5-nitrophenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



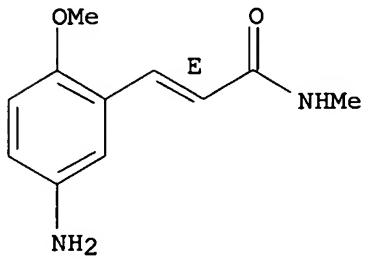
IT **288151-85-9P 288151-86-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of Ph ureas and thioureas as orexin receptor antagonists)
RN 288151-85-9 CAPLUS
CN 2-Propenamide, 3-(2-methoxy-5-nitrophenyl)-N-methyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 288151-86-0 CAPLUS
CN 2-Propenamide, 3-(5-amino-2-methoxyphenyl)-N-methyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1999:551731 CAPLUS
DOCUMENT NUMBER: 131:170173
TITLE: Preparation of arylacrylate esters as precursors for organoleptic compounds
INVENTOR(S): Anderson, Denise; Frater, Georg
PATENT ASSIGNEE(S): Givaudan Roure (International) S.A., Switz.
SOURCE: Eur. Pat. Appl., 16 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
EP 936211	A2	19990818	EP 1999-810036	19990119	<--
EP 936211	A3	19990825			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
SG 93823	A1	20030121	SG 1999-82	19990113	
ZA 9900567	A	19990726	ZA 1999-567	19990126	<--
CN 1227837	A	19990908	CN 1999-101847	19990202	<--
MX 9901281	A	20000731	MX 1999-1281	19990204	<--
BR 9900443	A	20000502	BR 1999-443	19990210	<--
AU 9916430	A1	19991021	AU 1999-16430	19990212	<--
AU 725999	B2	20001026			
JP 2000063328	A2	20000229	JP 1999-33906	19990212	<--
US 6096918	A	20000801	US 1999-249384	19990212	<--
PRIORITY APPLN. INFO.:			EP 1998-810114 A	19980213	

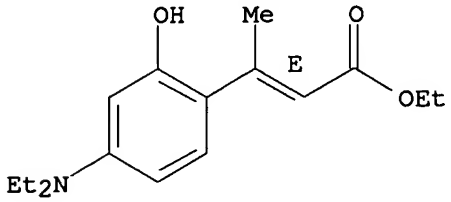
OTHER SOURCE(S): MARPAT 131:170173

AB (E)-RZZ1CO2R1 [R = OH or NHR6; R1 = H, (aromatic) hydrocarbyl, **heterocyclyl**, heteroaryl; R1 may be substituted by an ionic substituent; R6 = H, (un)saturated hydrocarbyl, aryl, etc.; Z = (un)substituted 1,2-phenylene or -naphthylene; Z1 = CR2:CH or CH:CR2; R2 = H, a straight or branched C1-C6 residue (sic), (un)substituted **heterocyclyl**, -aryl], which cyclize under use conditions to give coumarins having organoleptic and/or antimicrobial and/or optical brightening properties, were prepared Thus, 2-(HO)C6H4CHO was condensed with Ph3P:CMeCO2Et to give (E)-2-(HO)C6H4CH:CMeCO2Et.

IT **238402-44-3P**
RL: MOA (Modifier or additive use); SPN (Synthetic preparation); PREP

(Preparation); USES (Uses)
(preparation of arylacrylate esters as precursors for organoleptic compds.)
RN 238402-44-3 CAPLUS
CN 2-Butenoic acid, 3-[4-(diethylamino)-2-hydroxyphenyl]-, ethyl ester, (2E)-(9CI) (CA INDEX NAME)

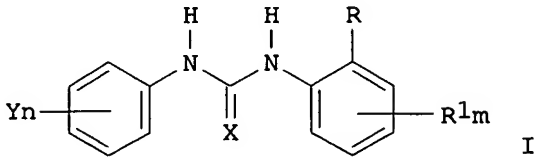
Double bond geometry as shown.



L5 ANSWER 3 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:479029 CAPLUS
DOCUMENT NUMBER: 129:122458
TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists
INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Hertzberg, Robert Philip; Rutledge, Melvin Clarence, Jr.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: U.S., 50 pp., Cont.-in-part of U.S. Ser. No. 641,990.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5780483	A	19980714	US 1996-701299	19960821 <--
US 5886044	A	19990323	US 1996-641990	19960320 <--
US 6211373	B1	20010403	US 1998-111663	19980708
PRIORITY APPLN. INFO.:			US 1995-390260 B2	19950217
			US 1996-641990 A2	19960320
			WO 1996-US2260 W	19960216
			US 1996-701299 A3	19960821

OTHER SOURCE(S): MARPAT 129:122458
GI



I

AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of ≤10 (sic); R1, Y = H, halo, NO2, cyano, (halo)alkyl, alkenyl, (halo)alkoxy, N3, HO, hydroxyalkyl, aryl, arylalkyl, aryloxy, arylalkoxy, heteroaryl, heteroarylalkyl, **heterocyclyl**, **heterocyclylalkyl**, **heterocyclylalkoxy**, arylalkenyl, heteroarylalkenyl, (un)substituted NH2, CONH2, or SO3H, etc.; m, n = 1-3],

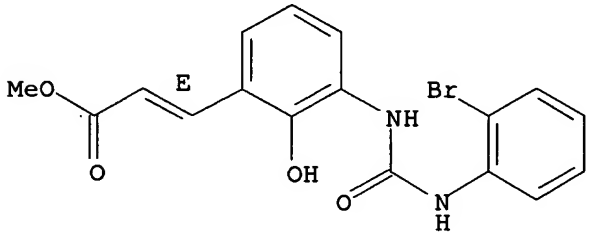
which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared Thus, Me 4-amino-3-hydroxybenzoate was added to a solution of Ph isocyanate in PhMe and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4-(methoxycarbonyl)phenyl]-N'-phenylurea.

IT **182499-23-6P 182499-25-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

RN 182499-23-6 CAPLUS

CN 2-Propenoic acid, 3-[3-[[[(2-bromophenyl)amino]carbonyl]amino]-2-hydroxyphenyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

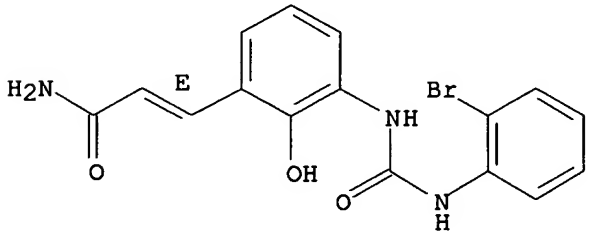
Double bond geometry as shown.



RN 182499-25-8 CAPLUS

CN 2-Propenamide, 3-[3-[[[(2-bromophenyl)amino]carbonyl]amino]-2-hydroxyphenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

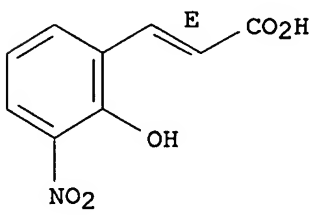


IT **86981-08-0P 182500-04-5P 182500-05-6P 182500-06-7P 182500-07-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

RN 86981-08-0 CAPLUS

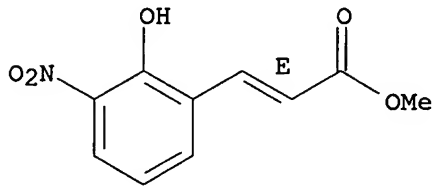
CN 2-Propenoic acid, 3-(2-hydroxy-3-nitrophenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



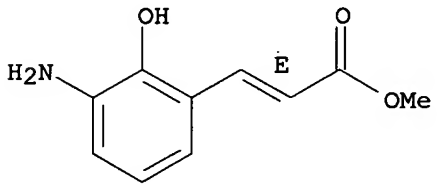
RN 182500-04-5 CAPLUS
CN 2-Propenoic acid, 3-(2-hydroxy-3-nitrophenyl)-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



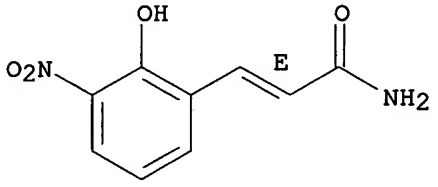
RN 182500-05-6 CAPLUS
CN 2-Propenoic acid, 3-(3-amino-2-hydroxyphenyl)-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



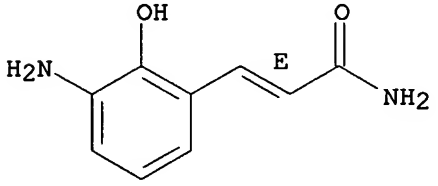
RN 182500-06-7 CAPLUS
CN 2-Propenamide, 3-(2-hydroxy-3-nitrophenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 182500-07-8 CAPLUS
CN 2-Propenamide, 3-(3-amino-2-hydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



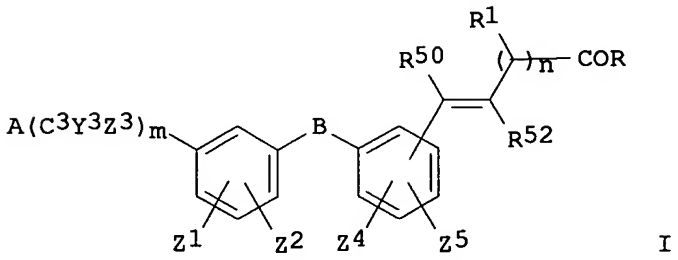
REFERENCE COUNT: 84 THERE ARE 84 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:679050 CAPLUS
DOCUMENT NUMBER: 127:346406
TITLE: Preparation of acylaminocinnamates and related compounds as integrin antagonists.
INVENTOR(S): Chen, Barbara B.; Chen, Helen Y.; Clare, Michael; Docter, Stephen H.; Khanna, Ish Kumar; Koszyk, Francis Jan; Malecha, James W.; Miyashiro, Julie M.; et al.
PATENT ASSIGNEE(S): G.D. Searle and Co., USA
SOURCE: PCT Int. Appl., 278 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 9736860	A1	19971009	WO 1997-US4462		19970325 <--
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG					
CA 2250690	AA	19971009	CA 1997-2250690		19970325 <--
EP 894084	A1	19990203	EP 1997-916111		19970325 <--
EP 894084	B1	20020626			
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI					
JP 2000510098	T2	20000808	JP 1997-532954		19970325 <--
AT 219764	E	20020715	AT 1997-916111		19970325
ES 2179318	T3	20030116	ES 1997-916111		19970325
AU 9723371	A1	19971022	AU 1997-23371		19970326 <--
PRIORITY APPLN. INFO.:			US 1996-14325P	P	19960329
			WO 1997-US4462	W	19970325

OTHER SOURCE(S): MARPAT 127:346406
GI



I

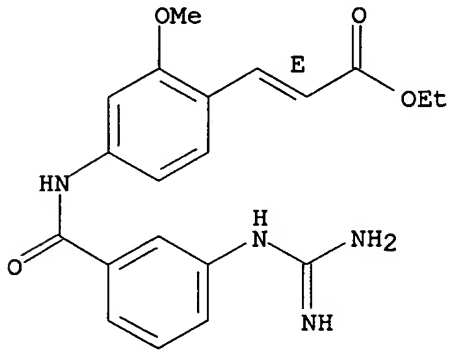
AB Title compds. [I; A = NR5C(Y1)NR7R8, NR5C(NR7)Y2; Y1 = NR2, O, S; R = XR3; R1 = H, alkyl, amino, acylamino, etc.; X = O, S, NR4; R2 = H, (substituted) alkyl, aryl, OH, alkoxy, cyano, NO2, amino, aminocarbonyl, alkenyl, alkynyl, etc.; R3, R4 = H, alkyl, alkenyl, alkynyl, haloalkyl, aryl, aralkyl, sugar residue, steroid residue, etc.; R5 = H, alkyl, alkenyl, alkynyl, PhCH2, PhCH2CH2; R7 = H, (substituted) alkyl, alkenyl, alkynyl, aralkyl, cycloalkyl, bicycloalkyl, aryl, acyl, etc.; R50 = H, alkyl, (substituted) aryl, etc.; R52 = H, acylamino, (substituted)

hydrazino; R2R7 = (substituted) **heterocyclyl**, heteroaryl; R7R8 = (substituted) **heterocyclyl**; Y2R7 = (substituted) **heterocyclyl**; Z1, Z2, Z3, Z5 = H, alkyl, OH, alkoxy, aryloxy, aralkoxy, halo, haloalkyl, haloalkoxy, NO2, amino, aminoalkyl, cyano, alkylsulfonyl, carboxyalkenyl, (fused) aryl, etc.; B = (CH2)pO, CH:CH, CH2CONH, CONH(CH2)p, CO2, SO2NH, etc.; m = 0-2; n = 0-3; p = 0-2]. Thus, 3-[2-methoxy-4-[[[3-[(1,2,3,4-tetrahydropyrimidin-2-yl)amino]phenyl]carbonyl]amino]phenyl]propionic acid trifluoroacetate (preparation given) antagonized αvβ3 with IC50 = 0.43 nM.

IT **198193-15-6P 198193-16-7P 198193-18-9P 198193-19-0P 198193-54-3P 198193-55-4P 198193-62-3P 198193-63-4P 198193-72-5P 198193-73-6P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acylaminocinnamates and related compds. as integrin antagonists)

RN 198193-15-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]benzoyl]amino]-2-methoxyphenyl]-, ethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

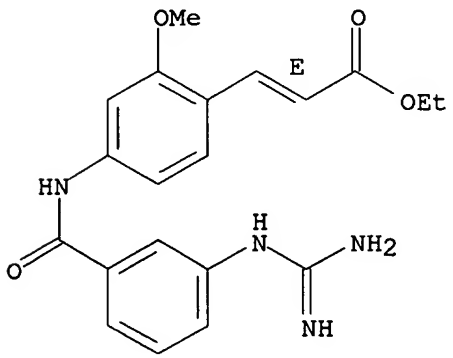


RN 198193-16-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]benzoyl]amino]-2-methoxyphenyl]-, ethyl ester, (E)-, trifluoroacetate (10:11) (9CI) (CA INDEX NAME)

CM 1

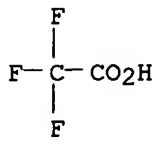
CRN 198193-15-6
CMF C20 H22 N4 O4

Double bond geometry as shown.



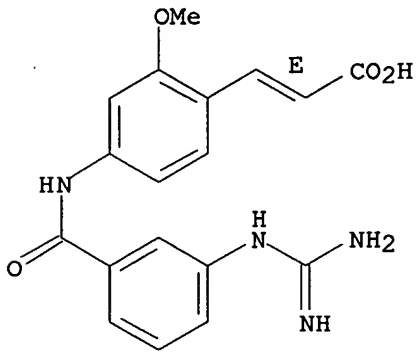
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 198193-18-9 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]benzoyl]amino]-2-methoxyphenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

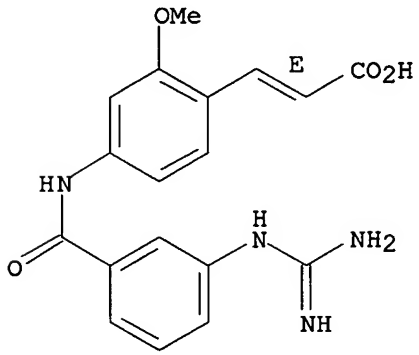


RN 198193-19-0 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]benzoyl]amino]-2-methoxyphenyl]-, (E)-, trifluoroacetate (5:6) (9CI) (CA INDEX NAME)

CM 1

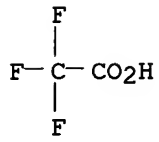
CRN 198193-18-9
CMF C18 H18 N4 O4

Double bond geometry as shown.



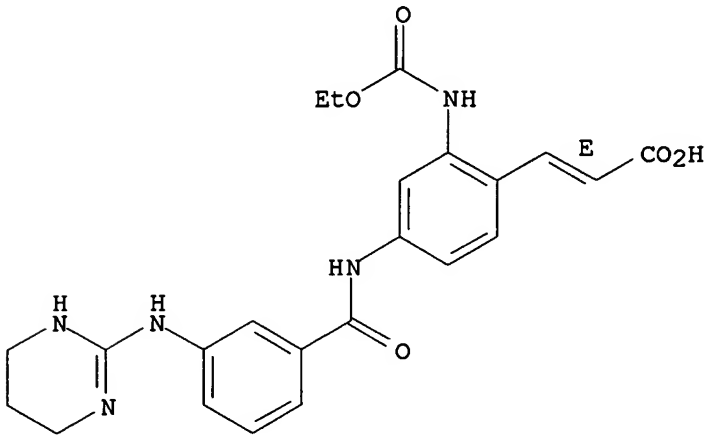
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 198193-54-3 CAPLUS
CN 2-Propenoic acid, 3-[2-[(ethoxycarbonyl)amino]-4-[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]benzoyl]amino]phenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

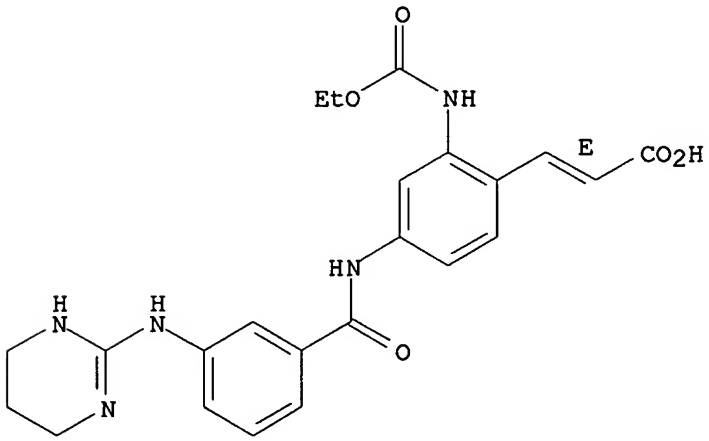


RN 198193-55-4 CAPLUS
CN 2-Propenoic acid, 3-[2-[(ethoxycarbonyl)amino]-4-[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]benzoyl]amino]phenyl]-, (E)-, trifluoroacetate (5:9) (9CI) (CA INDEX NAME)

CM 1

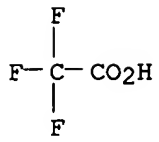
CRN 198193-54-3
CMF C23 H25 N5 O5

Double bond geometry as shown.



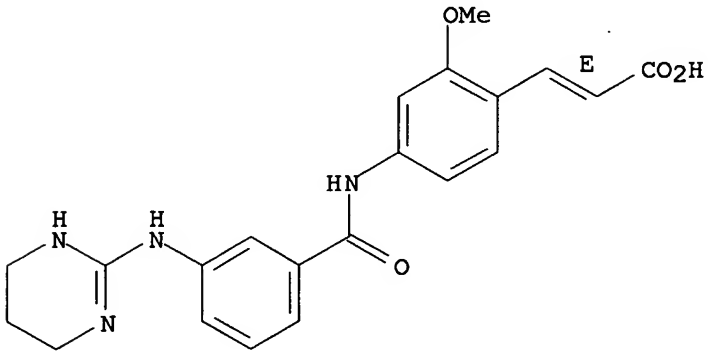
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 198193-62-3 CAPLUS
CN 2-Propenoic acid, 3-[2-methoxy-4-[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]benzoyl]amino]phenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

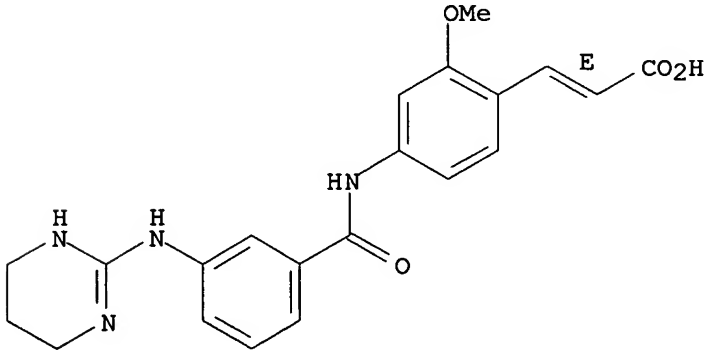


RN 198193-63-4 CAPLUS
CN 2-Propenoic acid, 3-[2-methoxy-4-[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]benzoyl]amino]phenyl]-, (E)-, trifluoroacetate (5:6) (9CI) (CA INDEX NAME)

CM 1

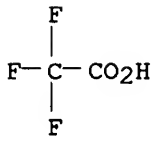
CRN 198193-62-3
CMF C21 H22 N4 O4

Double bond geometry as shown.



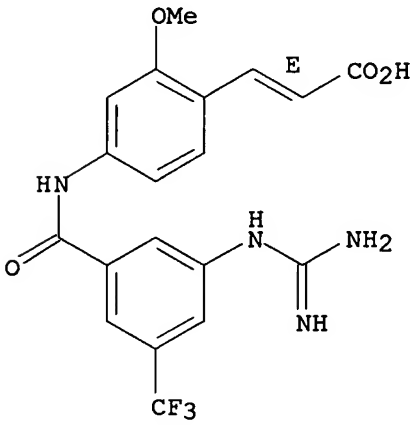
CM 2

CRN 76-05-1
CMF C2 H F3 O2



RN 198193-72-5 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]-5-(trifluoromethyl)benzoyl]amino]-2-methoxyphenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

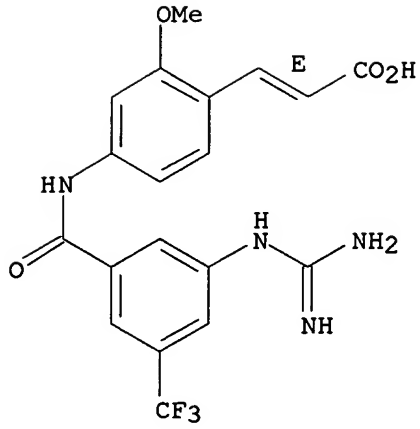


RN 198193-73-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[3-[(aminoiminomethyl)amino]-5-(trifluoromethyl)benzoyl]amino]-2-methoxyphenyl]-, (E)-, trifluoroacetate (2:3) (9CI) (CA INDEX NAME)

CM 1

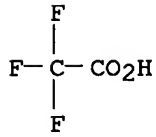
CRN 198193-72-5
CMF C19 H17 F3 N4 O4

Double bond geometry as shown.



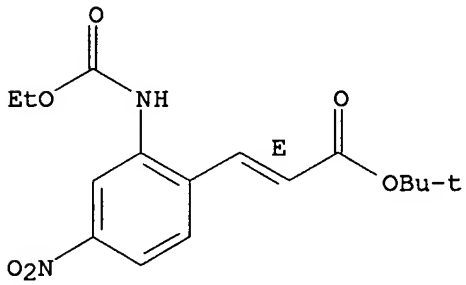
CM 2

CRN 76-05-1
CMF C2 H F3 O2



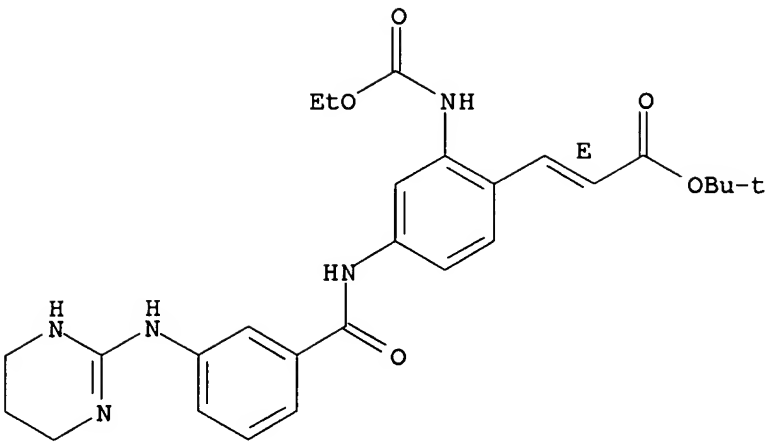
IT **198194-94-4P 198194-95-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of acylaminocinnamates and related compds. as integrin antagonists)
RN 198194-94-4 CAPLUS
CN 2-Propenoic acid, 3-[2-[(ethoxycarbonyl)amino]-4-nitrophenyl]-, 1,1-dimethylethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 198194-95-5 CAPLUS
CN 2-Propenoic acid, 3-[2-[(ethoxycarbonyl)amino]-4-[[3-[(1,4,5,6-tetrahydro-2-pyrimidinyl)amino]benzoyl]amino]phenyl]-, 1,1-dimethylethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L5 ANSWER 5 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1997:41948 CAPLUS
DOCUMENT NUMBER: 126:59875
TITLE: Preparation of beta-**heterocyclyl**-alpha, beta-unsaturated ketone derivatives as inhibitors of interleukin 1 production
INVENTOR(S): Tanaka, Masayuki; Okita, Makoto; Miyamoto, Mitsuaki; Kaneko, Toshihiko; Kawahara, Tetsuya; Akamatsu, Keishi; Chiba, Kenichi; Obaishi, Hiroshi; Sakurai, Hideki; Abe, Shinya; Kobayashi, Seiichi; Yamanaka, Takashi
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: PCT Int. Appl., 254 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9636608	A1	19961121	WO 1996-JP1330	19960520 <--
W: CA, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 08311032	A2	19961126	JP 1995-142394	19950518 <--
PRIORITY APPLN. INFO.:			JP 1995-142394 A	19950518

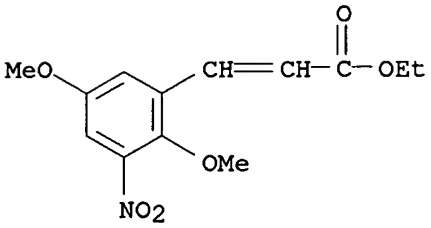
OTHER SOURCE(S): MARPAT 126:59875
GI For diagram(s), see printed CA Issue.
AB α,β-Unsatd. ketone derivs. represented by general formula RCH:CHCOR1 [R = Q, Q1; wherein Z = NH, O, S; ring B = an optionally substituted aromatic ring; R2 = H, halo, optionally halogenated lower alkyl, etc.; R3 = H, optionally halogenated lower alkyl, cycloalkyl optionally having heteroatom(s), alkoxyalkyl, optionally substituted aryl, optionally substituted heteroaryl, etc.; R1 = CR4R5R6; wherein R4, R5 = H, optionally halogenated lower alkyl, etc.; R6 = H, optionally halogenated lower alkyl, cycloalkyl optionally having heteroatom(s), optionally substituted aryl, optionally substituted heteroaryl, etc.] or pharmacol. acceptable salts thereof, which are useful for the prevention and treatment of interleukin 1 production-related diseases, e.g. inflammation, are prepared Thus, 1.68 g 7-ethyl-4-methoxymethoxy-3,5,8-trimethoxy-2-quinolinecarboxaldehyde and 1.0 g 3-hydroxy-3-methyl-2-butanone were dissolved in MeOH, treated with 0.21 g LiOH.H2O and heated at 50-60° for 1 h to give, after treatment of the product with 1 N aqueous HCl in EtOAc, the title quinolinylbutenone derivative (I; R7 = R10 = OMe, R8 = H, R9 = Et, R11 =

CMe2OH). The latter compound and I (R7 = R9 = R10 = H, R8 = Cl, R2 = R11 = Me) showed IC50 of 1.08 and <0.1 nM, resp., for inhibiting the production of interleukin 1α in human peripheral monocyte and 0.92 and <0.1 nM, resp., for inhibiting the production of interleukin 1β in human peripheral monocyte.

IT **185207-34-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of β- **heterocyclyl**-α, β-unsatd. ketone derivs. as inhibitors of interleukin 1 production)

RN 185207-34-5 CAPLUS

CN 2-Propenoic acid, 3-(2,5-dimethoxy-3-nitrophenyl)-, ethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 6 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

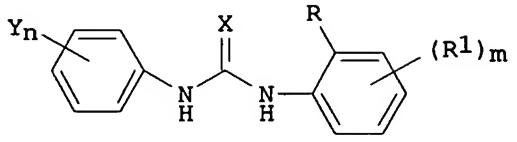
ACCESSION NUMBER: 1996:643902 CAPLUS
DOCUMENT NUMBER: 125:275430
TITLE: Preparation of N,N'-diphenylurea derivatives as interleukin-8 receptor antagonists
INVENTOR(S): Widdowson, Katherine Louisa; Veber, Daniel Frank; Jurewicz, Anthony Joseph; Rutledge, Melvin Clarence, Jr.; Hertzberg, Robert Philip
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 5
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9625157	A1	19960822	WO 1996-US2260	19960216 <--
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 809492	A1	19971203	EP 1996-906547	19960216 <--
R: BE, CH, DE, DK, FR, GB, IT, LI, NL				
JP 11503110	T2	19990323	JP 1996-525199	19960216 <--
CA 2432662	AA	19970821	CA 1996-2432662	19960821 <--
WO 9729743	A1	19970821	WO 1996-US13632	19960821 <--
W: AL, AM, AU, BB, BG, BR, CA, CN, CZ, EE, GE, HU, IL, IS, JP, KG, KP, KR, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9669007	A1	19970902	AU 1996-69007	19960821 <--
AU 725456	B2	20001012		
EP 896531	A1	19990217	EP 1996-929723	19960821 <--
R: AT, ES, GR, LU, SE, MC, PT, IE, SI, LT, LV, FI				

CN 1215990	A	19990505	CN 1996-180245		19960821	<--
JP 2000504722	T2	20000418	JP 1997-529318		19960821	<--
NZ 316710	A	20000526	NZ 1996-316710		19960821	<--
BR 9612779	A	20001024	BR 1996-12779		19960821	<--
CN 1539816	A	20041027	CN 2004-10032423		19960821	
US 6005008	A	19991221	US 1997-894291		19970815	<--
US 6211373	B1	20010403	US 1998-111663		19980708	
NO 9803737	A	19981014	NO 1998-3737		19980814	<--
US 6180675	B1	20010130	US 1999-240354		19990129	
PRIORITY APPLN. INFO.:			US 1995-390260	A2	19950217	
			WO 1996-US2260	W	19960216	
			US 1996-641990	A3	19960320	
			CA 1996-2245927	A3	19960821	
			US 1996-701299	A3	19960821	
			WO 1996-US13632	W	19960821	

OTHER SOURCE(S): MARPAT 125:275430

GI



I

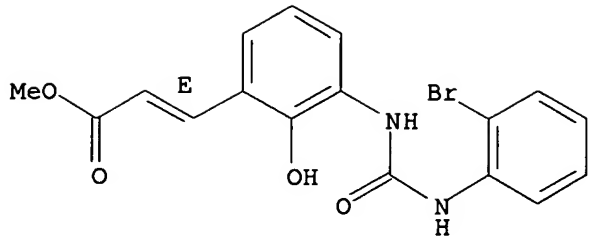
AB The title compds. [I; X = O, S; R = any functional moiety having an ionizable H and a pKa of ≤10; R1, Y = H, halo, NO2, cyano, C1-10 (halo)alkyl, C2-10 alkenyl, C1-10 (halo)alkoxy, N3, HO, C1-4 hydroxyalkyl, aryl, aryl-C1-4 alkyl, aryloxy, aryl-C1-4 alkoxy, heteroaryl, heteroarylalkyl, **heterocyclyl**, **heterocyclyl**-C1-4 alkyl, **heterocyclyl**-C1-4 alkoxy, aryl-C2-10 alkenyl, heteroaryl-C2-10 alkenyl, (un)substituted NH2, carbamoyl, or SO3H, etc.; m, n = 1-3], which are useful for the treatment of disease states mediated by the chemokine, interleukin-8 (IL-8) (no data), are prepared The chemokine-mediated disease is selected from psoriasis or atopic dermatitis, asthma, chronic obstructive pulmonary disease, adult respiratory distress syndrome, arthritis, inflammatory bowel disease, Crohn's disease, ulcerative colitis, septic shock, endotoxic shock, gram neg. sepsis, toxic shock syndrome, stroke, cardiac and renal reperfusion injury, glomerulo-nephritis, thrombosis, Alzheimer's disease, graft vs. host reaction, and allograft rejections. Thus, 1.19 mmol Me 4-amino-3-hydroxybenzoate was added to a solution of 1.19 mmol Ph isocyanate in toluene and the resulting mixture was stirred at .apprx.80° for 24-48 h to give 90% N-[2-hydroxy-4-(methoxycarbonyl)phenyl]-N'-phenylurea.

IT **182499-23-6P 182499-25-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)

RN 182499-23-6 CAPLUS

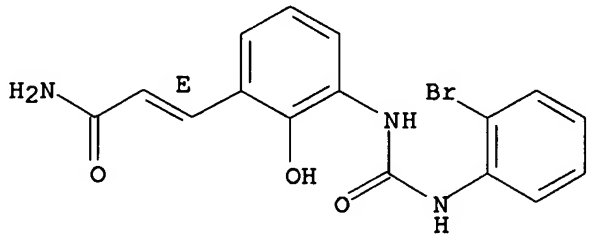
CN 2-Propenoic acid, 3-[3-[[[(2-bromophenyl)amino]carbonyl]amino]-2-hydroxyphenyl]-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



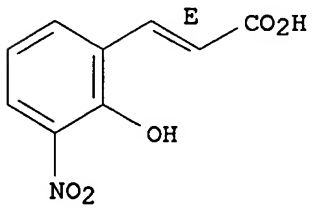
RN 182499-25-8 CAPLUS
CN 2-Propenamide, 3-[3-[[[(2-bromophenyl)amino]carbonyl]amino]-2-hydroxyphenyl]-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



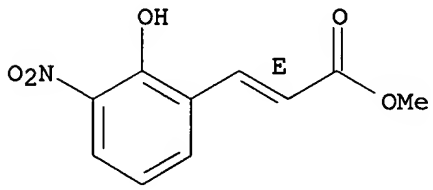
IT **86981-08-0P 182500-04-5P 182500-05-6P 182500-06-7P 182500-07-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N,N'-diphenylurea derivs. as interleukin-8 receptor antagonists for disease treatment)
RN 86981-08-0 CAPLUS
CN 2-Propenoic acid, 3-(2-hydroxy-3-nitrophenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



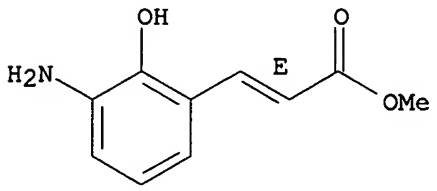
RN 182500-04-5 CAPLUS
CN 2-Propenoic acid, 3-(2-hydroxy-3-nitrophenyl)-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



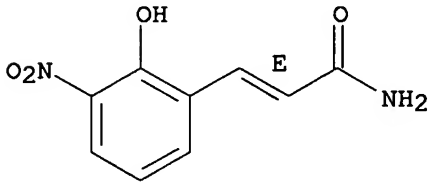
RN 182500-05-6 CAPLUS
CN 2-Propenoic acid, 3-(3-amino-2-hydroxyphenyl)-, methyl ester, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



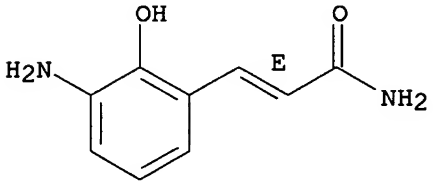
RN 182500-06-7 CAPLUS
CN 2-Propenamide, 3-(2-hydroxy-3-nitrophenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 182500-07-8 CAPLUS
CN 2-Propenamide, 3-(3-amino-2-hydroxyphenyl)-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



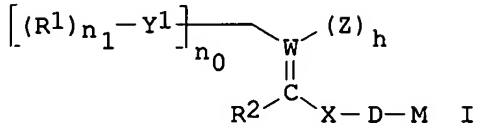
L5 ANSWER 7 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1993:244465 CAPLUS
DOCUMENT NUMBER: 118:244465
TITLE: Silver halide photographic light-sensitive material
INVENTOR(S): Matushita, Tetunori
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 74 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 508432	A1	19921014	EP 1992-106180	19920409 <--
EP 508432	B1	19980325		
R: DE, FR, GB, NL				

JP 04311952	A2	19921104	JP 1991-103584		19910410 <--
US 5266453	A	19931130	US 1992-866517		19920410 <--
PRIORITY APPLN. INFO.:			JP 1991-103584	A	19910410

OTHER SOURCE(S): MARPAT 118:244465

GI



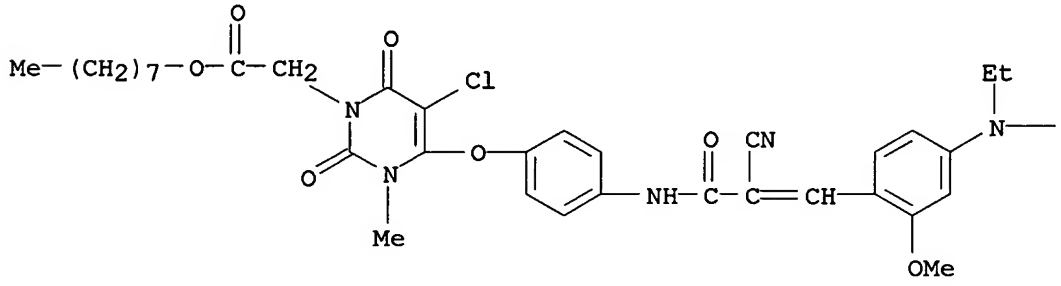
AB Photog. material with improved safelight property contains in ≥1 hydrophilic colloidal layer ≥1 filter dye which is irreversibly bleached during processing step. The filter dye comprises I (R1,R2 = H, or a substitutable) group; n0, n1, n2 = 0-1; h = 1-2; R1,R2,R3 = may together form a hydrocarbon or **heterocyclic** ring; Y1 = CO, CO(NR4), CS, C(N+R5R6), SO, SO2, C(CR7R8), R6CN, or C6CCR9 in [(R1)n1 Y1] when n1 = 1 and in Y1(R3)n2 when n2 = 1 in which R4-R9 = H or a substitutable group, Y1 = CN, NO2 in [(R1)nY1] when n1 = 0 and in Y1(R3)n2 when n2 = 0; x - divalent linkage; D = photog. dye residue; M = amphoteric group.

IT **146844-68-0**
RL: USES (Uses)
(photog. material with improved safelight property containing filter dye of)

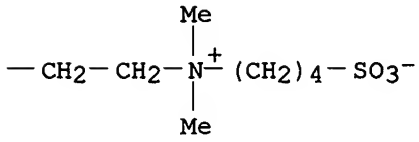
RN 146844-68-0 CAPLUS

CN 1-Butanaminium, N-[2-[[4-[3-[[4-[[5-chloro-1,2,3,6-tetrahydro-3-methyl-1-[2-(octyloxy)-2-oxoethyl]-2,6-dioxo-4-pyrimidinyl]oxy]phenyl]amino]-2-cyano-3-oxo-1-propenyl]-3-methoxyphenyl]ethylamino]ethyl]-N,N-dimethyl-4-sulfo-, inner salt (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

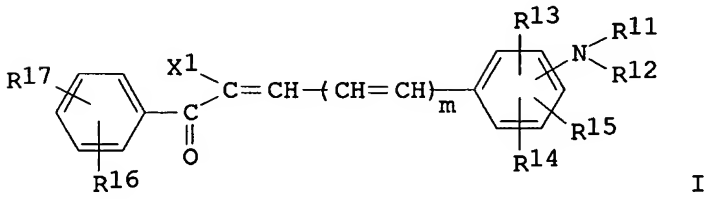


L5 ANSWER 8 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

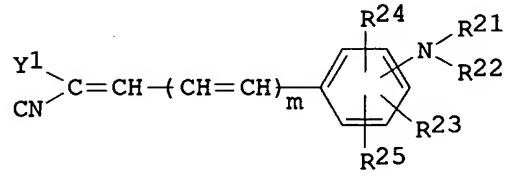
ACCESSION NUMBER: 1993:29821 CAPLUS
DOCUMENT NUMBER: 118:29821
TITLE: Photographic material containing quick bleachable dyes
INVENTOR(S): Kawashima, Yasuhiko; Yamauchi, Reiko; Kagawa, Nobuaki
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04116639	A2	19920417	JP 1990-237765	19900907 <--
PRIORITY APPLN. INFO.:			JP 1990-237765	19900907

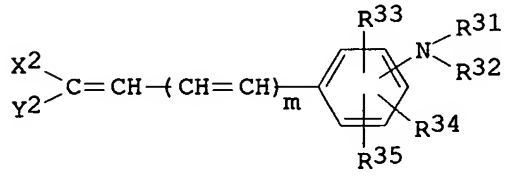
GI



I



II



III

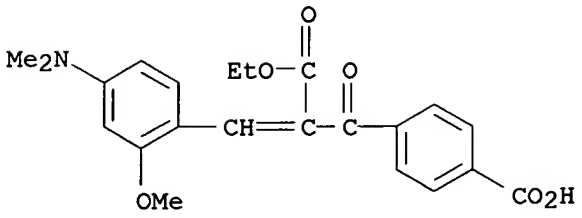
AB The title photog. material contains a dispersed fine solid powder of a compound selected from I, II and III [R1,2 = H, (cyclo)alkyl, alkenyl, aryl, **heterocyclyl**, acyl, sulfonyl; R1 and R2 may form a 5- or 6-membered ring; R3-5 = H, halo, alkyl, CO2H, alkoxycarbonyl, aryloxycarbonyl, amino, carbamoyl, sulfamoyl, NO2, CN, OH, alkoxy, SH, aryl, alkenyl; X1 = COR8, CONR8R9, CO2R8, SO2R8, SOR8, SO2NR8R9; R8,9 = H, (cyclo)alkyl, aryl, **heterocyclyl**, alkenyl; m = 0-2; Y1 = CN, CONR8R9, CO2R8, SO2R8, SOR8, SO2NR8R9; X2, Y2 = COR8R9, CO2R8, SO2R8, SOR8, SO2NR8R9].

IT **144806-78-0 144807-06-7 144807-09-0 144807-25-0**
RL: USES (Uses)
(bleachable dye, photog. material containing)

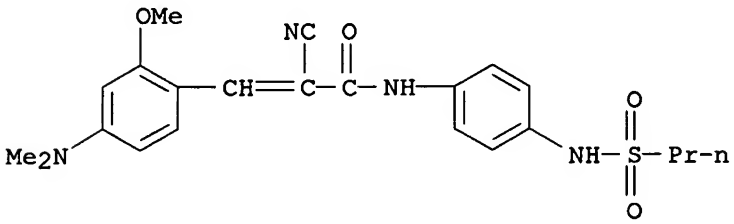
RN 144806-78-0 CAPLUS

CN Benzenepropanoic acid, 4-carboxy-α-[[4-(dimethylamino)-2-methoxyphenyl]methylene]-β-oxo-, α-ethyl ester (9CI) (CA INDEX

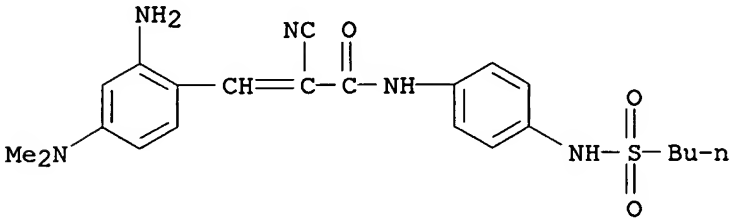
NAME)



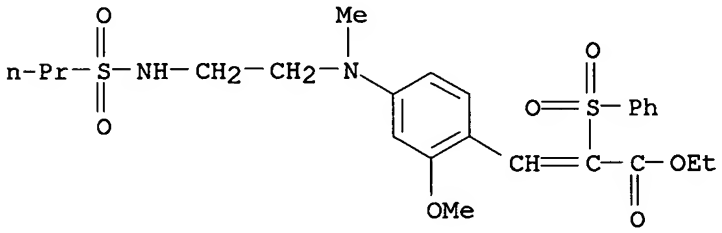
RN 144807-06-7 CAPLUS
CN 2-Propenamide, 2-cyano-3-[4-(dimethylamino)-2-methoxyphenyl]-N-[4-[(propylsulfonyl)amino]phenyl]- (9CI) (CA INDEX NAME)



RN 144807-09-0 CAPLUS
CN 2-Propenamide, 3-[2-amino-4-(dimethylamino)phenyl]-N-[4-[(butylsulfonyl)amino]phenyl]-2-cyano- (9CI) (CA INDEX NAME)

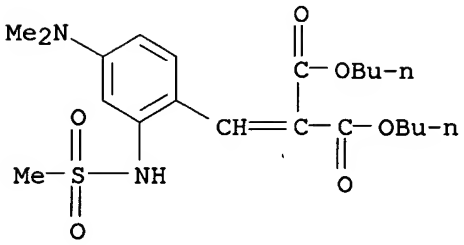


RN 144807-25-0 CAPLUS
CN 2-Propenoic acid, 3-[2-methoxy-4-[methyl[2-[(propylsulfonyl)amino]ethyl]amino]phenyl]-2-(phenylsulfonyl)-, ethyl ester (9CI) (CA INDEX NAME)



IT **144807-45-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and use of, as bleachable dye, photog. material containing)
RN 144807-45-4 CAPLUS
CN Propanedioic acid, [[4-(dimethylamino)-2-[(methylsulfonyl)amino]phenyl]met

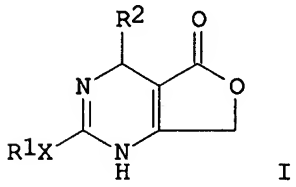
hylene]-, dibutyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 9 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:407953 CAPLUS
DOCUMENT NUMBER: 117:7953
TITLE: Preparation of 4,7-dihydrofuro[3,4-d]pyrimidin-5(1H)-one derivatives
INVENTOR(S): Rovnyak, George C.; Kimball, Spencer D.
PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA
SOURCE: Brit. UK Pat. Appl., 28 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2247236	A1	19920226	GB 1991-17865	19910819 <--
GB 2247236	B2	19940105		
US 5103006	A	19920407	US 1990-570664	19900821 <--
PRIORITY APPLN. INFO.:			US 1990-570664 A	19900821
OTHER SOURCE(S):	MARPAT 117:7953			

GI

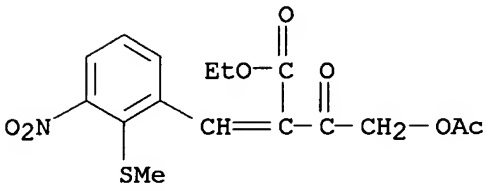


I

AB Title compds. I [X = O, S; R1 = alkyl, alkenyl, alkynyl, (alkyl)cycloalkyl, -aryl, -**heterocyclyl**, hydroxyalkyl, alkoxyalkyl, mercaptoalkyl, (substituted) amino, **heterocyclyl**, etc.; R2 = aryl, **heterocyclyl**] and salts thereof, useful as cardiovascular agents (no data), are prepared Et 4-(acetyloxy)-2-[[2-(methylthio)-3-nitrophenyl]methylene]-3-oxobutanoate (preparation given), 2-methyl-2-thiopseudourea sulfate and AcONa in DMF were heated for 6 h to give an Et (hydroxymethyl)pyrimidinecarboxylate derivative which in MeOH, DMSO and NaOH was stirred at room temperature for 1.5 h to give I [R1 = Me, X = S, R2 = 2,3-(MeS)(O2N)C6H3]; this was converted to its mono-HCl salt.

IT **141776-01-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)

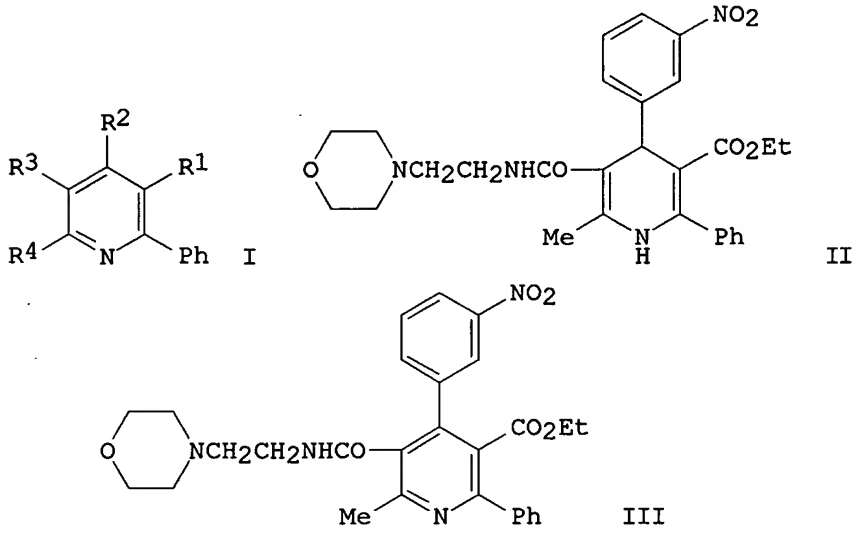
(preparation of, as intermediate in preparation of cardiovascular agents)
RN 141776-01-4 CAPLUS
CN Butanoic acid, 4-(acetyloxy)-2-[[2-(methylthio)-3-nitrophenyl]methylene]-3-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 10 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1992:106096 CAPLUS
DOCUMENT NUMBER: 116:106096
TITLE: Preparation of phenylpyridine derivatives for treatment of brain and heart ischemia
INVENTOR(S): Takasugi, Hisashi; Kuno, Atsushi; Sakai, Hiroyoshi
PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03223253	A2	19911002	JP 1990-17579	19900126 <--

PRIORITY APPLN. INFO.: JP 1990-17579 19900126
OTHER SOURCE(S): MARPAT 116:106096
GI

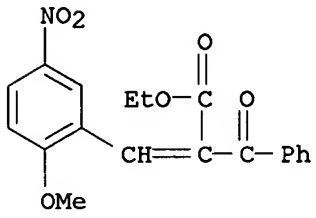


AB Phenylpyridine derivs. [I; R1 = CO2H, alkyl, cyano, alkylsulfonyl, acyl, etc.; R2 = cyano, NO2, halo, (alkyl- or alkoxy-substituted) aryl,

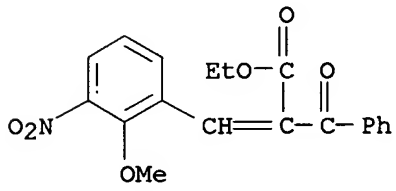
heterocyclyl; R3 = (esterified) CO2H, (substituted) carbamoyl, **heterocyclylcarbonyl**; R4 = alkyl] are prepared BF3-Et2O was added dropwise to a solution of 5 g Et 2-benzoyl-3-(3-nitrophenyl)acrylate in CH2Cl2 at room temperature, followed by a solution of 6.6 g 3-amino-N-(2-morpholinoethyl)crotonamide in CH2Cl2, the mixture was refluxed, the reaction mixture adjusted to pH 9, washed, dried, filtered to give dihydropyridine II, which was refluxed with MnO2 to 1.1 g pyridine derivative III. Also prepared were 33 addnl. I, which restored ATP content by 71.8-93.2% in ischemic guinea pigs at 1 + 10-5 g/mL.

IT **138994-19-1P 138994-20-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antiischemic compds.)

RN 138994-19-1 CAPLUS
CN Benzenepropanoic acid, α-[(2-methoxy-5-nitrophenyl)methylene]-β-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 138994-20-4 CAPLUS
CN Benzenepropanoic acid, α-[(2-methoxy-3-nitrophenyl)methylene]-β-oxo-, ethyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 11 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1991:428892 CAPLUS
DOCUMENT NUMBER: 115:28892
TITLE: Preparation of phenylalkan(en)oic acids as leukotriene B4 antagonists.
INVENTOR(S): Konno, Mitoshi; Nakae, Takahiko; Hamanaka, Nobuyuki
PATENT ASSIGNEE(S): Ono Pharmaceutical Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 205 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 405116	A2	19910102	EP 1990-109294	19900516 <--
EP 405116	A3	19920415		
EP 405116	B1	19951206		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

CA 2019335	AA	19901227	CA 1990-2019335	19900507 <--
CA 2019335	C	20000801		
JP 03261752	A2	19911121	JP 1990-123146	19900515 <--
JP 07039369	B4	19950501		
EP 619296	A1	19941012	EP 1994-108324	19900516 <--
EP 619296	B1	19970312		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

EP 652208	A1	19950510	EP 1994-118144	19900516 <--
EP 652208	B1	19980114		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE

AT 131154	E	19951215	AT 1990-109294	19900516 <--
ES 2083396	T3	19960416	ES 1990-109294	19900516 <--
AT 150006	E	19970315	AT 1994-108324	19900516 <--
ES 2102097	T3	19970716	ES 1994-108324	19900516 <--
AT 162181	E	19980115	AT 1994-118144	19900516 <--
ES 2114117	T3	19980516	ES 1994-118144	19900516 <--
US 5086065	A	19920204	US 1990-524521	19900517 <--
KR 143404	B1	19980715	KR 1990-7107	19900518 <--
US 5155104	A	19921013	US 1991-760043	19910913 <--
US 5256686	A	19931026	US 1992-921342	19920729 <--
JP 06072947	A2	19940315	JP 1993-131187	19930507 <--
JP 08019040	B4	19960228		
US 5457122	A	19951010	US 1993-90456	19930713 <--
US 5795914	A	19980818	US 1995-462815	19950605 <--
US 6001877	A	19991214	US 1998-81549	19980520 <--

PRIORITY APPLN. INFO.:	JP 1989-164213	A	19890627
	JP 1989-310545	A	19891201
	JP 1990-1799	A	19900109
	EP 1990-109294	A3	19900516
	US 1990-524521	A3	19900517
	US 1991-760043	A3	19910913
	US 1992-921342	A3	19920729
	US 1993-90456	A3	19930713
	US 1995-462815	A3	19950605

OTHER SOURCE(S): MARPAT 115:28892

GI For diagram(s), see printed CA Issue.

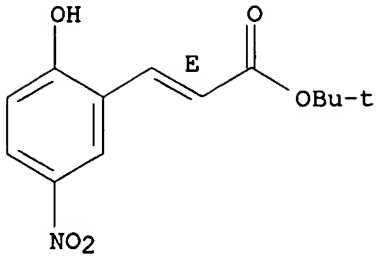
AB Title compds. I (A = NHCO, O, NHSO2, CO, CH2, CHOH; W = C1-13 alkylene, phenylene, C6H4CH2; R1 = H, C1-4 alkyl, HO2C, (unsatd.) 4-7-membered N-**heterocyclyl**, carbamoyl, HOCH2; AWR1 = Q1, Q2, Q3, etc.; Y = CH2CH2, CH:CH; D = hydroxyalkenylene, etc.), are prepared tert-Bu 3-[1-[6-(4-methoxyphenyl)hex-5(E)-enyl]oxy-4-(4-carboxybutanamido)benzen-2-yl]propionate (preparation starting from 2-hydroxy-5-nitrobenzaldehyde given) in THF/Et3N was treated with ClCO2Et at -10° and then with Me2NH to give the dimethylamide derivative which was hydrolyzed in HCO2H to give the title acid-amide E-II. II inhibited binding of 3H-LTB4 to human polymorphonuclear leukocyte LTB4 receptors with IC50 = 0.045 μM. A tablet formulation containing 3-[1-[6-(4-methoxyphenyl)hex-5(E)-enyl]oxy-3-(4-carboxybutyl)oxybenzen-2-yl]propionic acid is given.

IT **134577-68-7P 134577-76-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of LTB4 antagonists)

RN 134577-68-7 CAPLUS

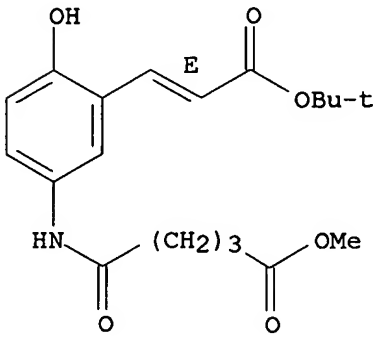
CN 2-Propenoic acid, 3-(2-hydroxy-5-nitrophenyl)-, 1,1-dimethylethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



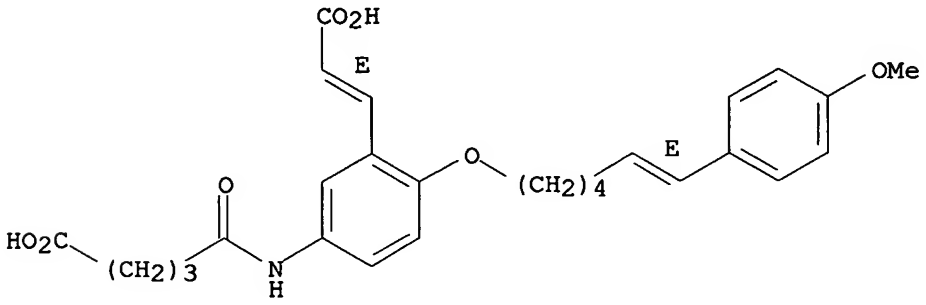
RN 134577-76-7 CAPLUS
CN Pentanoic acid, 5-[[3-[3-(1,1-dimethylethoxy)-3-oxo-1-propenyl]-4-hydroxyphenyl]amino]-5-oxo-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT **134578-32-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as LTB4 antagonist)
RN 134578-32-8 CAPLUS
CN Pentanoic acid, 5-[[3-(2-carboxyethenyl)-4-[[6-(4-methoxyphenyl)-5-hexenyl]oxy]phenyl]amino]-5-oxo-, (E,E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

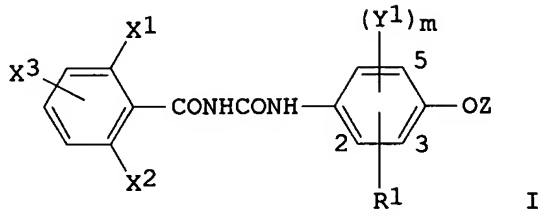


L5 ANSWER 12 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1987:515373 CAPLUS
DOCUMENT NUMBER: 107:115373
TITLE: Pesticidal 1-(4-aryloxyphenyl)-3-benzoylureas; processes for their preparation, and pesticidal compositions and methods employing them
INVENTOR(S): Caruso, Andrew James
PATENT ASSIGNEE(S): Union Carbide Corp., USA

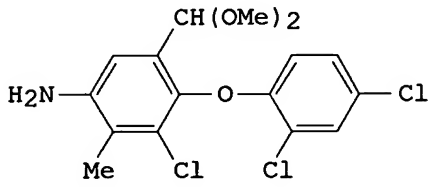
SOURCE: Eur. Pat. Appl., 62 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
EP 220840	A2	19870506	EP 1986-307457		19860929	<--
EP 220840	A3	19880323				
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE						
JP 62111961	A2	19870522	JP 1986-228521		19860929	<--
ZA 8607420	A	19870527	ZA 1986-7420		19860929	<--
AU 8663260	A1	19870402	AU 1986-63260		19860930	<--
BR 8604732	A	19870630	BR 1986-4732		19860930	<--
PRIORITY APPLN. INFO.:			US 1985-781382	A	19850930	
			US 1986-895364	A	19860811	

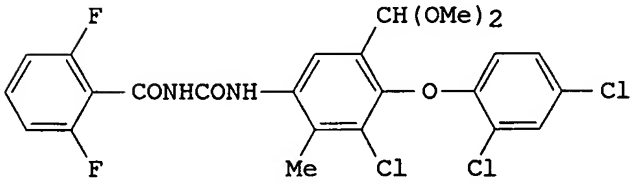
GI



I



II



III

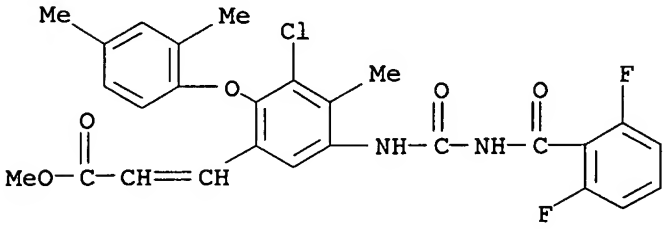
AB The title compds. [I; X1 = halo; X2, X3 = H, halo; Y1 = halo, alkyl, alkoxy, NO2, cyano; m = 0-2; R1 = CHO, CO2H or ester, hydroxyalkyl, alkoxyalkyl, acyloxyalkyl, alkenyl, alkanoyl, (a)cyclic acetal, dithioacetal, hemithioacetal; m = 2 and R1 is not at 2- or 6-position when R1 = CO2H or ester; Z = (un)substituted (un)saturated mono- or bicyclic fused ring system (latter has 1 benzene ring and one carbo- or **heterocyclic** 5- or 6-membered ring containing a CO group and/or 1 or 2 O or S atoms] are prepared as pesticides. Neat 2,6-F2C6H3CONCO (23.63 mmol) was added to a solution of phenoxyaniline derivative II (23.63 mmol) in PhMe. The mildly exothermic reaction precipitated 90% (phenoxyphenyl)benzoylurea III, which was 71-100% lethal against Spodoptera eridania at 100 ppm (spray) on bean leaves in laboratory expts.

IT **110123-43-8P**

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as pesticide)

RN 110123-43-8 CAPLUS

CN 2-Propenoic acid, 3-[3-chloro-5-[[[(2,6-difluorobenzoyl)amino]carbonyl]amino]-2-(2,4-dimethylphenoxy)-4-methylphenyl]-, methyl ester (9CI) (CA INDEX NAME)



L5 ANSWER 13 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1981:603820 CAPLUS

DOCUMENT NUMBER: 95:203820

TITLE: Addition of **heterocyclic** CH acids to the carbon-nitrogen double bond of azomethines

AUTHOR(S): Pavlenko, N. I.; Marshtupa, V. P.; Klyuev, N. A.; Baskunov, B. P.

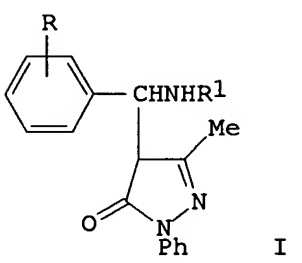
CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, 340055, USSR

SOURCE: Khimiya Geterotsiklicheskikh Soedinenii (**1981**), (8), 1088-93
CODEN: KGSSAQ; ISSN: 0453-8234

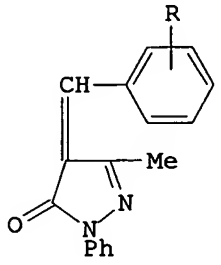
DOCUMENT TYPE: Journal

LANGUAGE: Russian

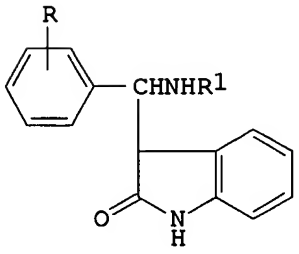
GI



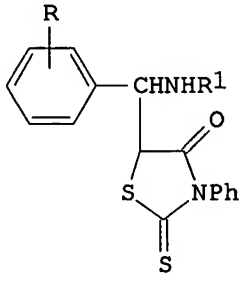
I



II



III



IV

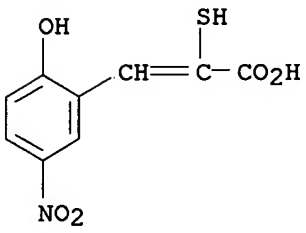
AB Aminomethylation of 1-phenyl-3-methyl-5-pyrazolone by RC6H4CH:NR1 (R = H, 3-NO2, 3-OH, 4-MeO, 2-MeO, 4-Me, 2-HO, 4-Cl; R1 = 4-IC6H4, 4-BrC6H4,

3-BrC6H4, Ph, Me, 7-quinolyl) gave 10-70% addition products I. Treatment of I (R = H, R1 = 4-BrC6H4; R = 4-MeO, R1 = Ph) with acid gave II in 40 and 53% yield, resp. Indolones III (R = 2-OH, 4-OH, 4-Me, 4-MeO, 4-NO2, 4-F, 4-Cl, H, R1 = Et, Ph, 4-O2NC6H4, 4-ClC6H4, 4-BrC6H4, 4-IC6H4) and thiazolidines IV (R = 3-NO2, 4-OH, 4-Me2N, 4-Br, 4-F, 4-NO2, H; R1 = Ph, 3-O2NC6H4, PhOC6H4, Me) were prepared similarly in 31-92% yield. Acid treatment of III gave the corresponding benzylideneindolones. Treatment of IV with OH- gave 15-75% RC6H4CH:C(SH)CO2H.

IT **79787-80-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 79787-80-7 CAPLUS

CN 2-Propenoic acid, 3-(2-hydroxy-5-nitrophenyl)-2-mercapto- (9CI) (CA INDEX NAME)



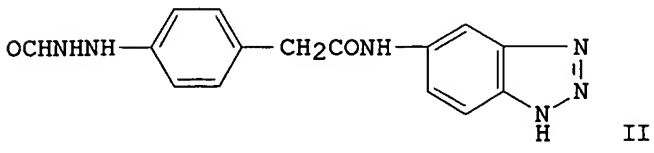
L5 ANSWER 14 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1980:568271 CAPLUS
DOCUMENT NUMBER: 93:168271
TITLE: Hydrazide nucleating agents, methods employing them and photographic materials containing them
INVENTOR(S): Sidhu, Jasbir; Simons, Michael John; Baigrie, Brian Devlin; Mijovic, Miroslav Vasa; Southby, David Thomas
PATENT ASSIGNEE(S): Kodak Ltd., UK
SOURCE: Brit. UK Pat. Appl., 14 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2011391	A	19790711	GB 1977-52302	19771215 <--
GB 2011391	A	19790711	GB 1978-48701	19781215 <--
GB 2011391	B2	19820324		

PRIORITY APPLN. INFO.: GB 1977-52302 A 19771215

GI



II

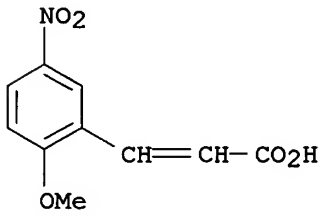
AB 3,4-RR1C6H3NHNHCOR2 [I; R = H, R3(Z)nZ1(Z2)m(CH2)x [R3 = group which renders I capable of being adsorbed to the surface of a photog. Ag halide grain; Z, Z2 = divalent aliphatic or aromatic hydrocarbon or

heterocyclic moiety; Z1 = NR4CO (R4 = H, alkyl), NR4SO2, O2C, CONR4, SO2NR4, CO2; n, m = 0, 1; x = 1-4]; R1 = R3(O)y (y = 0, 1), R6(CH2)zO (R6 = H, optionally substituted alkyl or aryl, z = 1-4); R2 = H, optionally substituted alkyl or aryl] were prepared Thus, the amide II was prepared (20%) from 5-aminobenzotriazole by stirring it in DMF at room temperature overnight with p-OCHNHNHC6H4CH2CO2H in the presence of dicyclohexylcarbodiimide. I are useful as photog. nucleating agents. They are adsorbed strongly to Ag halide grains and function at lower pH than previously described. A preferred use of I is in photog. dye image transfer systems both of the peel-apart and integral type.

IT **69447-75-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate in preparation of benzotriazolyl(formylhydrazino aryl)propionamide)

RN 69447-75-2 CAPLUS

CN 2-Propenoic acid, 3-(2-methoxy-5-nitrophenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 15 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

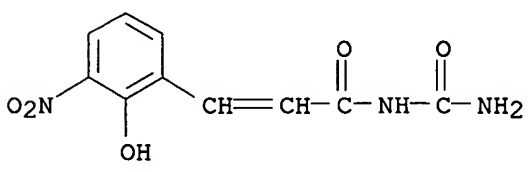
ACCESSION NUMBER: 1977:552324 CAPLUS
DOCUMENT NUMBER: 87:152324
TITLE: Phosphonium salts and ylides based on chloroacetylurea
AUTHOR(S): Kushnir, V. N.; Shevchuk, M. I.; Dombrovskii, A. V.
CORPORATE SOURCE: Chernovits. Gos. Univ., Chernovtsy, USSR
SOURCE: Zhurnal Obshchei Khimii (**1977**), 47(8), 1715-21
CODEN: ZOKHA4; ISSN: 0044-460X
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB Reaction of H2NCONHCOCH2Cl with Ph3P gave 94% H2NCONHCOCH2P+Ph3Cl- which on treatment with NH4OH gave 87% H2NCONHCOCH:PPh3 (I). Treating I with RX gave 85-94% H2NCONHCOCHRP+Ph3X- (R = Br, iodo, Me, Me3Si; X = halo) which on dehydrohalogenation gave 67-82% H2NCONHCOCR:PPh3. Treating I with R1CHO gave 77-99% of 16 H2NCONHCOCH:CHR1 (R1 = Ph, substituted phenyl, 2-furyl, 2-quinolyl, etc.) which on bromination gave H2NCONHCOCHBrCHBrR1.

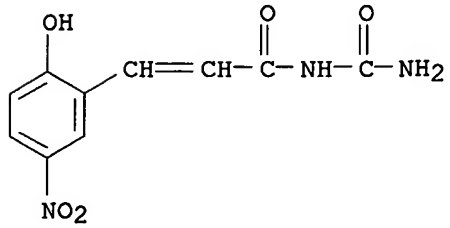
IT **62879-66-7P 62879-67-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 62879-66-7 CAPLUS

CN 2-Propenamide, N-(aminocarbonyl)-3-(2-hydroxy-3-nitrophenyl)- (9CI) (CA INDEX NAME)



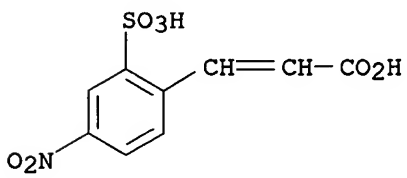
RN 62879-67-8 CAPLUS
CN 2-Propenamide, N-(aminocarbonyl)-3-(2-hydroxy-5-nitrophenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 16 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1976:91660 CAPLUS
DOCUMENT NUMBER: 84:91660
TITLE: **Heterocyclic** styryl compounds
INVENTOR(S): Tonegawa, Kakuji; Jono, Shuichi; Fujino, Tomizo
PATENT ASSIGNEE(S): Osaka Seika Chemical Industries, Ltd., Japan
SOURCE: Jpn. Tokkyo Koho, 8 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50022051	B4	19750728	JP 1966-6348	19660202 <--
PRIORITY APPLN. INFO.:			JP 1966-6348	19660202

GI For diagram(s), see printed CA Issue.
AB Styryl fluorescent whitening agents I (R = H, SO3Na; R1 = H, Me; R2 = H, Cl, Me or (R2R3) = benzo; A is an optionally substituted benzene, naphthalene, or **heterocyclic** ring) are prepared by triazolizing the appropriate amino azo coupling product. For example, 2-(p-aminostyryl)-5-methylbenzoxazole [6661-12-7] was diazotized and coupled with 4,1-H2NC10H6SO3Na [130-13-2] and the product triazolized with NaOCl in aqueous pyridine to give I (R = R1 = R3 = H, R2 = Me, A = 4-sulfo-1,2-naphtho) [58307-08-7], fluorescence λmax 422 mμ. The following I were similarly prepared (R-R3, A, and fluorescence max in mμ given): H, H, H, H, 4-sulfo-1,2-naphtho, 420; H, H, Me, H, 6-sulfo-1,2-naphtho, 440; H, H, Me, H, 7-sulfo-1,2-naphtho, 416; H, H, Me, H, 5-sulfo-1,2-naphtho, 449; H, H, Cl, H, 4-sulfo-1,2-naphtho, 421; H, Me, Me, H, 6,8-disulfo-1,2-naphtho, 445; 3-SO3Na, H, H, H, 1,2-naphtho, 429; and 9 others.
IT **58307-05-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminocresol)
RN 58307-05-4 CAPLUS
CN 2-Propenoic acid, 3-(4-nitro-2-sulfophenyl)- (9CI) (CA INDEX NAME)



L5 ANSWER 17 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1974:84703 CAPLUS
DOCUMENT NUMBER: 80:84703
TITLE: Yellow coumarin dyes
INVENTOR(S): Sato, Katsunobu
PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

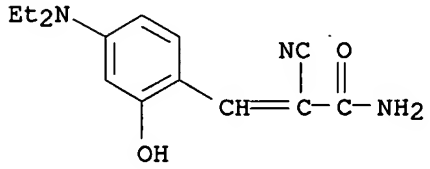
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 48080122	A2	19731026	JP 1972-11985	19720201 <--
JP 51042611	B4	19761117		

PRIORITY APPLN. INFO.: JP 1972-11985 A 19720201

AB Coumarin dyes (I, R1, R2 = H, alkyl, or cycloalkyl, or R1, R2, and N form a **heterocyclic** group; X = S, NH, or NR3, R3 = alkyl, aryl, or aralkyl; A = benzene or naphthalene ring with or without substituents except CO2H and SO3H) are prepared through condensation reactions. The dyes are useful for dyeing acetate, polyester, or polyamide fibers in fluorescent yellow shades with good fastness. Thus, NCCH2CONH2 was treated with 4,2-(Et2N)(HO)C6H3CHO in MeOH containing piperidine at room temperature to give 4,2-(Et2N)(HO)C6H3CH:C(CN)CONH2 which was treated with o-(H2N)2C6H4 in DMF at 100-10.deg. to give a yellow dye (I, R1 = R2= Et, X = NH, A = benzene ring) [27425-55-4]. Similarly prepared were 2 other I.

IT **42005-48-1P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

RN 42005-48-1 CAPLUS
CN 2-Propenamide, 2-cyano-3-[4-(diethylamino)-2-hydroxyphenyl]- (9CI) (CA INDEX NAME)



L5 ANSWER 18 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1972:128826 CAPLUS
DOCUMENT NUMBER: 76:128826
TITLE: Oxazolylacetic acid derivatives and oxazolylcoumarins for dyeing organic fibers
INVENTOR(S): Harnisch, Horst
PATENT ASSIGNEE(S): Farbenfabriken Bayer A.-G.
SOURCE: Ger. Offen., 80 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

DE 2030507	A	19720105	DE 1970-2030507	19700620 <--
DE 2030507	B2	19740919		
DE 2030507	C3	19750522		
CH 717157	A4	19760630	CH 1971-7157	19710513 <--
CH 587833	A	19770513	CH 1973-16185	19710513 <--
CH 585250	A	19770228	CH 1973-16186	19710613 <--
BE 768722	A1	19711103	BE 1971-104800	19710618 <--
NL 7108436	A	19711222	NL 1971-8436	19710618 <--
FR 2099247	A5	19720310	FR 1971-22352	19710618 <--
GB 1329042	A	19730905	GB 1971-28704	19710618 <--
GB 1329043	A	19730905	GB 1972-38453	19710618 <--
AT 310707	B	19731010	AT 1971-5278	19710618 <--
AT 310743	B	19731010	AT 1972-6152	19710618 <--
JP 50023028	B4	19750805	JP 1971-43359	19710618 <--
US 3985763	A	19761012	US 1973-369124	19730612 <--
JP 50069380	A2	19750610	JP 1974-99075	19740830 <--
JP 51006266	B4	19760226		
JP 51000526	A2	19760106	JP 1974-99076	19740830 <--
JP 51042125	B4	19761113		

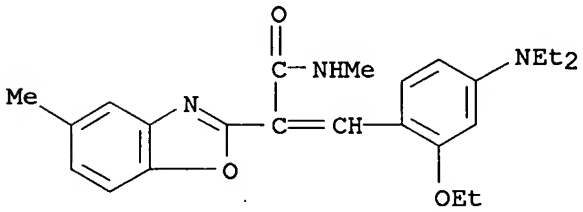
PRIORITY APPLN. INFO.: DE 1970-2030507 A 19700620
DE 1970-2058877 A 19701130
US 1971-154652 A1 19710618

AB Oxazoles [I, A represents benzene, naphthalene, or dibenzofuran ring; R = H, alkyl, cyclohexyl, aralkyl, aryl; R1 = H, alkyl, cyclohexyl, aralkyl, aryl, or (RR1N) = **heterocyclic** ring] were prepared by reaction of o-aminophenols with NCCH2CONRR1 and treated with 4-(dialkylamino)salicylaldehydes to give oxazolylcoumarins (II, R = Me, Et), fluorescent dyes for natural and synthetic fibers. For example, a mixture of o-H2NC6H4OH and NCCH2CONH2 was heated under N 30 min at 140-60.deg., 15 min at 150-60.deg., and 1 hr at 170.deg. to give 2-(2-benzoxazolyl)acetamide [34564-12-0]. Similarly, 46 other I were prepared A mixture of NCCH2CO2Et and MeO(CH2)3NH2 was heated 30 min at 60.deg., 3,4-H2N(HO)C6H3Me added, and the mixture heated 6 hr at 180.deg. to give N-(3-methoxypropyl)-5-methyl-2-benzoxazoleacetamide which (without isolation) was refluxed 20 hr with 4,2-Et2N(HO)C6H3CHO and iso-PrOH in the presence of piperidine to give 7-(diethylamino)-3-(5-methyl-2-benzoxazolyl)coumarin [34564-13-1], dyeing nylon-6 fabric a fast, brilliant greenish yellow shade. Similarly, 13 other II were prepared

IT **35773-52-5P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

RN 35773-52-5 CAPLUS

CN 2-Benzoxazoleacetamide, α-[[4-(diethylamino)-2-ethoxyphenyl]methylene]-N,5-dimethyl- (9CI) (CA INDEX NAME)



L5 ANSWER 19 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1944:41982 CAPLUS
DOCUMENT NUMBER: 38:41982
ORIGINAL REFERENCE NO.: 38:6288b-i,6289a-c
TITLE: Nitrogen **heterocycles**. LI. A new linear

benzodipicolone, 2,6-dimethyl-1,5-anthrazoline (2,7-dimethylpyrido[2,3-g]quinoline)

AUTHOR(S): Ruggli, Paul; Brandt, Fritz

SOURCE: Helvetica Chimica Acta (**1944**), 27, 274-91
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 38:41982

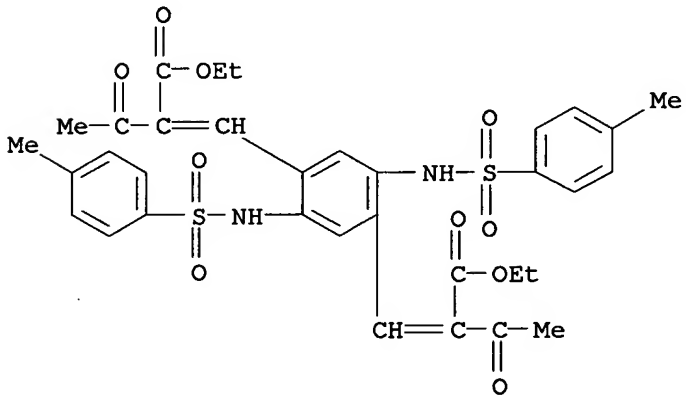
AB cf. C. A. 37, 1714.8. The successful use of 4,6-diaminoisophthalaldehyde for the previous synthesis of 1,8-anthrazoline derivs. (C. A. 32, 562.7) suggested the use of the corresponding 2,5-diaminoterephthalaldehyde (I) as a starting material for the preparation of derivs. of a new linear benzodipicoline, 2,7-dimethylpyrido[2,3-g]quinoline (II). Attempts to prepare I through 2,5-dichloroterephthalaldehyde (III) from 2,5-dichloro-p-xylene (IV) are briefly described though the yields and purity of the products left so much to be desired that a more successful approach was made through the corresponding 2,5-dibromoterephthalaldehyde (V). The chlorination of 50 g. p-xylene in the presence of 5 g. Fe powder in the dark at 12-15° in 3 hrs. and crystallization of the product from MeOH gave 43 g. (50%) of IV, m. 70-1°. Chlorination of the side-chain by passing dry Cl into 20 g. IV in 12 g. C6H2Cl4 at 120-30° with illumination gave 16.8 g. of 1,4-bis(dichloromethyl)-2,5-dichlorobenzene (VI), m. 72.5-4.0°, saponified by heating at 150-70° with concentrated H2SO4 for 20 min. The crude product, m. 144°, was purified through the dianil, C20H14Cl2N2, m. 213-140°, saponified by refluxing with 10% HCl and recrystd. from PhNO2 to give yellow needles of III, m. 157-8°. Other chlorination products including 2,3,5,6-tetrachloro-p-xylene, m. 216.5-17.0°; 1,4-bis (chloromethyl)-2,3,5,6-tetrachlorobenzene, m. 174.5-5.0° (dianil, C20H16Cl4N2, m. 170°); 1,4-bis(trichloromethyl)-2,5-dichlorobenzene, m. 193°. Bromination of 25 g. IV at 180 with 92 g. Br for 3.5 hrs. and crystallization of the product from CHCl3 yielded 40 g. of 1,4-bis(dibromomethyl)-2,5-dichlorobenzene, m. 127.5-8.0°. The bromination of 20 g. of p-xylene at 10-15° in the presence of a trace of iodine with 21.1 cc. Br and recrystn. of the crude product from alc. gave 44 g. of 2,5-dibromo-p-xylene (VII), m. 73.5-4.0°. Bromination of the side chain by adding in 5 hrs. 42.5 cc. Br to 50 g. VII at 120° and recrystn. of the crude product from 1100 cc. of boiling AcOEt yielded 78-81 g. (71-4%) of light yellow needles of α,α,α',α',2,5-hexabromo-p-xylene (VIII), m. 160-2. A mixture of 50 g. VIII and 250 cc. of H2SO4.H2O was heated at 130-40° and 25 mm. for 1 hr. The cooled solution was diluted with 1 kg. of ice and the crude product (26 g., m. 180-5°) was recrystd. from 250 cc. AcOH, producing 21.1 g. (84%) of V, m. 189-190.5°; dianil, m. 234.5-5.0°; tetraacetamide, m. above 305°. A mixture of 10 g. V with 1 g. Cu powder, 1 g. CuBr, 1 g. K2CO3, 18 g. of p-MeC6H4SO2NH2 and 40 cc. PhNO2 was heated at 140° and treated with 14 g. K2CO3 in 2 hrs. at 150-5°. After 3 hrs. at 160° the reaction mass was worked up and the crude product was recrystd. from AcOH and PhNO2, yielding 52-4% of 2,5-di-p-tolylsulfonamidoterephthalaldehyde (IX), C22H20N2O6S2, m. 241-3° (decomposition); dianil, m. 297° (decomposition). Condensation of 5 g. IX with 25 cc. AcCH2CO2Et at 70 in the presence of 12 drops of piperidine and crystallization from alc. gave 90% of di-Et 2,5-bis(p-tolylsulfonamido)terephthalylidenediacetoacetate (X), C34H36N2O10S2, m. 216-17° (decomposition). Treatment of 1.5 g. X with 5 cc. concentrated H2SO4 at 27-32° (not over 40) gave a one-sided ring-closure with the formation of Et 2-methyl-3-carbeth oxy-6-amino-7-quinoline(methyleneacetoacetate) (XI), m. 219-20°; picrate, m. 215-20° (decomposition). Treatment of 5 g. X with 20 cc. H2SO4 for 1 hr. below 95° saponified the ester group and gave 1.9 g.

of 2-methyl-3-carboxy-6-amino-7-quinoline(methyleneacetoacetic acid) (XII) which on further treatment with concentrated H2SO4 at 98-100° underwent further ring closure to 2,7-dimethylpyrido[2,3-g]quinoline-3,8-dicarboxylic acid (XIII), m. 320° (decomposition), also similarly prepared from X and XI. Decarboxylation of 1 g. XIII by adding it portionwise in 5 min. to 12 cc. quinoline at 215° containing 0.2 g. Cu powder and 0.2 g. CuCrO2, followed by removal of the quinoline with steam distillation and recrystn. of the crude product from alc., gave 0.2 g. (30%) of needles of II, C14H12N2, m. 238-9° (decomposition); picrate, m. 263° (decomposition); dibenzylidene derivative, m. 267°; bis(p-dimethylaminobenzylidene) derivative, m. above 340°. Treatment of 0.5 g. IX with 5 cc. PhCOMe at 190-7° for 1.5 hrs. and recrystn. of the product from alc. and PhNO2 produced greenish yellow leaflets of 2,7-diphenylpyrido[2,3-g]quinoline, m. 284-5°. From 100 g. p-xylene, the main products were 123 g. aldehyde (V), 100 g. sulfonamide (IX), 105 g. condensation product (X), 25 g. dicarboxylic acid (XIII) and, finally, 5 g. II.

IT **857619-45-5**, Acetoacetic acid, α,α'-[2,5-bis(p-tolylsulfonamido)terephthalylidene]bis-, diethyl ester
(preparation of)

RN 857619-45-5 CAPLUS

CN Acetoacetic acid, α,α'-[2,5-bis(p-tolylsulfonamido)terephthalylidene]bis-, diethyl ester (4CI) (CA INDEX NAME)



L5 ANSWER 20 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1940:12844 CAPLUS

DOCUMENT NUMBER: 34:12844

ORIGINAL REFERENCE NO.: 34:1986a-i,1987a

TITLE: Nitrogen **heterocycles**. XLVI. 4,6-Diaminoisophthalaldehyde. 3

AUTHOR(S): Ruggli, Paul; Frey, Hugo

SOURCE: Helvetica Chimica Acta (**1939**), 22, 1413-27
CODEN: HCACAV; ISSN: 0018-019X

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB The 3,6-dicarboxylic ester produced by the addition of 2 mols. AcCH2CO2Et to 4,6-diaminoisophthalaldehyde (I) was saponified to the free acid which was decarboxylated by heating with Cu in quinoline at 160-230° for 20 min. The resulting 2,7-dimethylbenzodipyridine (II) was converted into the hexa-Br derivative which was transformed by heating with oleum to the crude benzodipyridine-2,7-dicarboxylic acid (III). A mixture of 0.25 g. III, 2 cc. of 10% NH4OH and 2 cc. alc. was triturated, diluted with 20 cc. H2O and heated. The NH3-free product was diluted with 10 cc. H2O and boiled

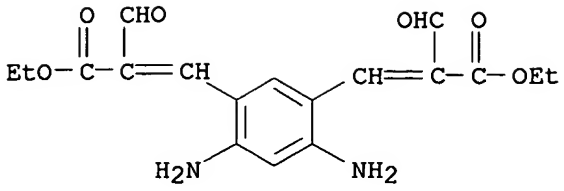
with 0.5 g. $AgNO_3$ in 10 cc. H_2O. The crude Ag salt (0.45 g.) was boiled with 70 cc. MeOH and 0.4 g. MeI for 1 h., filtered and concentrated to 20 cc., yielding 0.2 g. (70%) of yellow needles of di-Me benzodipyridine-2,7-dicarboxylate, $C_{16}H_{12}N_2O_4$, m. 272° (with darkening). Decarboxylation of III gave benzodipyridine (IV); perchlorate, m. 268° (explosive on rapid heating); MeI derivative, m. above 200° (decomposition). Reduction of 0.2 g. IV in 5 cc. of boiling AmOH with 0.35 g. Na and recrystn. from alc. gave octahydrobenzodipyridine, m. 111.5°, identified through the di-NO and di-Ac derivs., m. 179° (decomposition) and 143°, resp. Reduction of II with Na in AmOH gave as main product a resin which was converted into a colorless crystalline octahydro-2,7-dimethylbenzodipyridine diperchlorate, $C_{14}H_{22}Cl_2N_2O_8$, m. 285-6° (decomposition). The resinous free base yielded 2 isomeric di-NO derivs., m. 164.5 and 151.5-2.0°, resp. Condensation of 0.2 g. II with 0.5 g. of p-$Me_2NC_6H_4CHO$ at 170-5° in the presence of 10 drops of piperidine produced 0.45 g. of orange-red 2,7-bis(p-dimethylaminostyryl)benzodipyridine, $C_{32}H_{30}N_4$, m. about 340° (with darkening), dissolving in HCl to give violet, blue, green and yellow solns. with increasing acid concns. Condensation of II with o-$C_6H_4(CO_2Et)_2$ by heating in the presence of Na for 14 h. at 100° gave a scarlet crystalline powder which on sulfonation dyed wool and silk bluish red in an acid bath. A unilateral condensation of 0.6 g. I with 6 cc. $AcCH_2CO_2Et$ occurred on heating in the presence of 9 drops of piperidine for 30 min. at 170°. The impure 3-acetyl-6-formyl-7-aminocarbostyril yielded yellow crystals of a pure Ac derivative, $C_{14}H_{12}N_2O_4$, m. 320-40° (decomposition). Treatment of 1 g. I in 100 cc. alc. at 30° with 14 g. of dry $OHCCHNaCO_2Et$, boiling for 1 h. after standing for 3 days, filtering off the brown amorphous precipitate (V), adding 1 cc. H_2O and standing for 8 days gave a Na salt which was dissolved in 50 cc. H_2O, acidified with 10% HCl and recrystd. from dioxane, yielding di-Et 2,6-diaminoisophthalaldiformylacetate, $C_{18}H_{20}N_2O_6$, m. 250° (decomposition). V was dissolved in H_2O, filtered and precipitated with dilute HCl.

The amorphous product (0.06 g.) was decarboxylated by heating in vacuo with 0.3 g. BaO and 0.5 g. Cu at 150° to yield a bright yellow sublimate of IV. Condensation of I with excess cyclohexanone in the presence of piperidine produced 2,3,6,7-bis (tetramethylene)-benzodipyridine, $C_{20}H_{20}N_2$, m. 250-1° (with darkening); dipicrate, m. 195° (decomposition). A mixture of 8 g. I in 150 cc. alc., 24 cc. $PhCH_2CN$ and 12.5 cc. of 30% NaOH was heated for 30 min. on the steam bath. Working up and purification through the di-HCl salt gave a free base (VI), $C_{24}H_{18}N_4$, m. 301°; tetra-Ac derivative, $C_{32}H_{26}N_4O_4$, m. 238.5-9.5° (decomposition). Saponification of VI with HCl produced a carboxyl derivative, $C_{24}H_{18}N_2O_3$, which gave a Na salt and a mono-Ac derivative, m. 365°. Condensation of 4 g. of 4,6-dinitroisophthalaldehyde with 8.4 g. of dry $PhCH(Na)CO_2H$ by heating with 34 cc. Ac_2O and 1.2 g. $ZnCl_2$ for 40 h. at 80° gave a powdery dicarboxylic acid which was esterified through the Ag salt to di-Me 4,6-dinitroisophthalalbis(phenylacetate), $C_{26}H_{20}N_2O_8$, m. 152.5-3.5°. Condensation of methazonic acid (VII) with o-$H_2NC_6H_4CHO$ yields 3-nitroquinoline and similarly a cold mixture of VII and I in the presence of a min. of HCl gave 20% of yellow-orange needles of a compound $C_{16}H_{14}N_6O_5$, m. 290° (decomposition), of undetd. composition

IT **857578-13-3**, m-Benzenediacrylic acid, 4,6-diamino-α,α'-diformyl-, diethyl ester
(preparation of)

RN 857578-13-3 CAPLUS

CN m-Benzenediacrylic acid, 4,6-diamino-α,α'-diformyl-, diethyl ester (4CI) (CA INDEX NAME)



L5 ANSWER 21 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1939:8734 CAPLUS
DOCUMENT NUMBER: 33:8734
ORIGINAL REFERENCE NO.: 33:1325a-i,1326a
TITLE: Nitrogen **heterocycles**. XXXV. 4,6-Dinitro- and diaminoisophthalaldehydes. 2. lin-Benzodi-α-picoline and benzodipyridine
AUTHOR(S): Ruggli, Paul; Hindermann, Peter; Frey, Hugo
SOURCE: Helvetica Chimica Acta (**1938**), 21, 1066-83
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

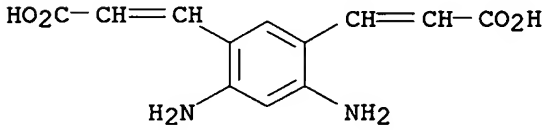
AB cf. C. A. 32, 3394.4. Dinitroisophthalaldehyde (I) (7 g.) in 40 cc. pyridine was warmed to 60°. CO2 and nitrous fumes developed, the temperature rose to 100° and the reaction ended in 45 min. Recrystn. of the resulting 4.8 g. of brown powder gave yellow leaflets, C25H18N2O6, m. above 300°. Other reactions of I with barbituric acid, indandione and methylphenylpyrazolone are cited. The product (0.5 g.) of the reaction between 7 g. I and CH2N2 (C. A. 31, 4287.9) is now considered to be 4,6-dinitrophenylene-1,3-diethylene oxide; C10H8N2O6, m. 153-4°, converted by HCl in pyridine to the corresponding 4,6-dinitrophenylene-1,3-diethylene chlorohydrin, C10H10Cl2N2O6, m. 150-1°. Boiling 2 g. Et diaminophenylenediacrylate (C. A. 31, 4287.9) with 30 cc. concentrated HCl for 15 min. gave 1.2-1.4 g. of impure 4,6-diaminophenylene-1,3-diacrylic acid HCl salts (II), converted by heating with a 20-fold excess of Ac2O at 120° to the mono-Ac derivative, C14H14N2O5, m. 320° (decomposition). Refluxing with 80 parts Ac2O for 50 min. produced the di-Ac compound, C16H16N2O6, m. 320° (decomposition). The mother liquors of the above saponification yielded yellow matted needles of 7-aminocarbostyril-6-acrylic acid, C12H10N2O3, m. above 300°. Heating 0.5 g. II with 25 cc. concentrated HCl in a bomb-tube for 5 h. at 160° gave, by double ring-closure, 2,7-dihydroxybenzodipyridine, C12H8N2O2, charring above 400°. Most condensations run more smoothly with diaminoisophthalaldehyde (III) than with I, on account of the sensitivity of the latter to alkaline condensation agents. Thus, refluxing 0.65 g. III in 50 cc. alc. and 1 g. barbituric acid in 30 cc. H2O for 10 min. produced 1.4 g. of fine, crystalline orange powder, 4,6-diaminoisophthalaldibarbituric acid, C16H12N6O6, charring above 300°. It is remarkable that no further ring-closure between the adjacent CO and NH2 groups takes place as in the condensation of o-H2NC6H4CHO with barbituric acid. In the presence of 10 drops of KOH in MeOH 0.5 g. III condensed with 5 g. of p-MeOC6H4Ac at 150° to give 0.6 g. of 2,7-di(p-methoxyphenyl)benzodipyridine, C26H20N2O2, m. 268-9°. Condensation of III (2.5 g.) with 10 g. AcCH2Ac in the presence of 15 drops of piperidine in a bomb-tube at 180-90° for 1.5 h. gave 3.5 g. of 2,7-dimethyl-3,6-diacetylbenzodipyridine dihydrate, C18H16N2O2.2H2O, m. 213-15°, converted by heating with Ac2O for 1 h. into an addition compound, C18H16N2O2.Ac2O which, on warming, gave the free base; dioxime, C18H18N4O2, m. 255-7°. III condensed with BzCH2CO2Et by 1-sided ring condensation to 3-benzoyl-6-aldehydo-7-aminocarbostyril, C17H12N2O3, m. 278-9° (decomposition); Ac derivative, C19H14N2O4, m. about 320° (decomposition). The ester resulting from the

condensation of III with AcCH2CO2Et in the presence of alc. NaOH (C. A. 31, 4287.9) was saponified and decarboxylated by heating 10 g. of the ester with 75 cc. concentrated HCl in a Durobax bomb-tube (70 cm. by 2.2 cm.; capacity, 270 cc.) up to 130° in 1.0-1.5 h. and for 2 h. at 130°. The crude product gave a high-melting polymer, C14H12N2.2H2O, m. 268°, and 2.8 g. of benzodi-α-picoline (IV), C14H12N2, m. 196-7°; dipicrate, m. 220° (decomposition); monoperchlorate, m. 228-30° (decomposition); diperchlorate, m. 318° (decomposition); chromate; MeI compound, sintering at 244°; dibenzal derivative, C28H20N2, m. 279°; difural derivative, C24H16N2O2, m. 271.5-2.5° (decomposition). Bromination of 4 g. IV in 80 cc. AcOH and 20 g. anhydrous AcONa at 70° with 18.5 g. Br in 40 cc. AcOH with stirring gave 12 g. (90%) of the hexa-Br derivative (V), C14H6Br6N2, m. 190-2° (decomposition), converted by heating with 15% oleum for 50 min. into the corresponding dicarboxylic acid (VI). A mixture of 0.6 g. VI, 2.5 g. Naturkupfer C, 1.8 g. anhydrous Ba(OH)2 and 1.8 g. BaO was sublimed in vacuo at 230-40° and yielded 45% (1.8 g.) of a yellow crystalline sublimate, m. 159-63°. The crude was dissolved in 15 cc. CHCl3 (distilled over K2CO3), filtered and shaken out with 2 cc. of 10% NaOH and with 4 lots of H2O (3 cc.). After drying over MgSO4, treating with charcoal and evaporating, the residue (0.11 g.) was recrystd. from 8 cc. H2O to give snow-white needles of lin-benzodipyridine (1,8-diazaanthracene) , C12H8N2, m. 164.5-5.0°; dipicrate, m. 262° (darkening).

IT **857578-15-5**, m-Benzenediacrylic acid, 4,6-diamino-
(hydrochlorides)

RN 857578-15-5 CAPLUS

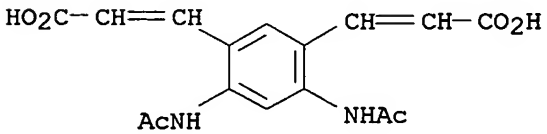
CN m-Benzenediacrylic acid, 4,6-diamino- (4CI) (CA INDEX NAME)



IT **857578-17-7**, m-Benzenediacrylic acid, 4,6-diacetamido-
857578-20-2, m-Benzenediacrylic acid, 4-acetamido-6-amino-
(preparation of)

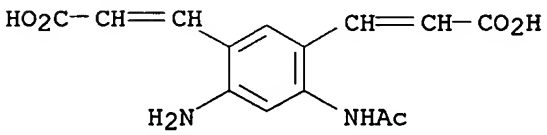
RN 857578-17-7 CAPLUS

CN m-Benzenediacrylic acid, 4,6-diacetamido- (4CI) (CA INDEX NAME)



RN 857578-20-2 CAPLUS

CN m-Benzenediacrylic acid, 4-acetamido-6-amino- (4CI) (CA INDEX NAME)

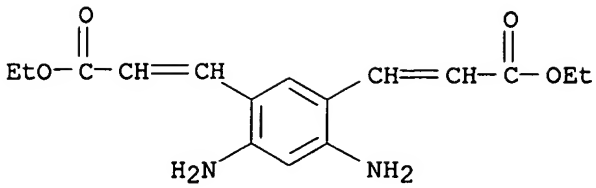


L5 ANSWER 22 OF 22 CAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1937:30573 CAPLUS
DOCUMENT NUMBER: 31:30573
ORIGINAL REFERENCE NO.: 31:4287i,4288a-f
TITLE: Nitrogen **heterocycles**. XXVIII. 4,6-Dinitro-and diaminoisophthalaldehyde. 1
AUTHOR(S): Ruggli, Paul; Hindermann, Peter
SOURCE: Helvetica Chimica Acta (**1937**), 20, 272-82
CODEN: HCACAV; ISSN: 0018-019X
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB 4,6-Dinitro-1,3-xylene (100 g.) and 150 g. p-NOC6H4NMe2 were boiled 8 h. in 500 cc. EtOH containing 100 g. anhydrous Na2CO3. Extraction of the crude product with 1.5 l. H2O and then 3 times with 350 cc. Me2CO left 57% of condensation product (I), 100 g. of which was shaken 24 h. with 620 cc. C6H6 (II) and 620 cc. HNO3 (d. 1.12). After filtering off the p-NH2C6H4NMe2.HNO3, the II layer was separated, and concentrated to 100 cc., when 4,6-dinitroisophthalaldehyde (III) (dianil, m. 164.5-65°; disemicarbazone, m. above 360° (decomposition)) crystallized III condenses with compds. containing an active CH2 group. Thus 1.5 g. III in 10 cc. pyridine (IV) was added to 3 g. barbituric acid in 90 cc. hot H2O. After long standing addition of dilute H2SO4 precipitated 4,6-dinitroisophthalaldibarbituric acid. CH2N2 (from 23 g. NO(Me)NCO2Et) in 200 cc. ether was poured over 7 g. III and left 15 h. in the ice box. Long fractional crystallization of the precipitate from EtOH gave 4,6-dinitro-1,3-diacetylbenzene, m. 153-4°. III (20 g.), 100 g. (HO2C)2CH2 and 60 cc. IV were warmed 48 h. at 50-5° and then 2 h. at 100°. Addition of 300 cc. 10% H2SO4 gave 68% of 4,6-dinitrophenylene-1,3-diacrylic acia, m. 216°, after purification through the Et ester (V), m. 116°, and saponification with H2SO4 in dilute AcOH. Reduction of 18 g. V with Rupe's Ni catalyst (VI) gave 14 g. di-Et 4,6-diaminophenylene-1,3-diacrylate, m. 195-6° (di-Ac derivative, m. 244-5°). Reduction of III with VI was unsuccessful. III (16 g.) in 600 cc. EtOH and 360 cc. concentrated NH4OH was dropped with strong stirring during 15 min. into 368 g. FeSO4 in 800 cc. H2O containing a few drops of 10% HCl warmed on the water bath. The Fe precipitate was extracted 15 h. in a Soxhlet with Me2CO (VII) and the residue after removal of VII, boiled with H2O and filtered. On strong chilling 84% of 4,6-diaminoisophthalaldehyde (VIII), m. 208°, separated; dioxime, m. 219-20°; disemicarbazone, chars above 360°; monophenylhydrazone, m. 275-6° (decomposition); diphenylhydrazone, m. 337° (decomposition); mono-Ac derivative, from VIII and Ac2O in the cold for 3 days, m. 270-2°; di-Ac derivative, prepared hot, m. 280-2°. VIII (0.5 g.) in 5 cc. MeCOPh containing 3-4 drops 10% MeOH-KOH at 100° for 10 min. gave, on precipitation with 50% EtOH, 70% of 2,7-diphenyl-lin-m-benzodipyridine, m. 216-17° (dipicrate, m. 270° (decomposition)). Similar condensation of VIII with AcCH2CO2Et gave di-Et 2,7-dimethylbenzodipyridine-3,6-dicarboxylate, m. 166-7°.

IT **857578-14-4**, m-Benzenediacrylic acid, 4,6-diamino-, diethyl ester
857578-16-6, m-Benzenediacrylic acid, 4,6-diacetamido-, diethyl ester
(preparation of)

RN 857578-14-4 CAPLUS
CN m-Benzenediacrylic acid, 4,6-diamino-, diethyl ester (4CI) (CA INDEX NAME)



RN 857578-16-6 CAPLUS
CN m-Benzenediacrylic acid, 4,6-diacetamido-, diethyl ester (4CI) (CA INDEX NAME)